

# On the Eigenfunctions of Many-Particle Systems in Quantum Mechanics\*

TOSIO KATO

*University of Tokyo and New York University*

## 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] by the writer, in which the fundamental properties, in particular the self-adjointness, of the Hamiltonian operator of such a system has been investigated.<sup>1</sup>

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,<sup>2</sup> and 2) that they have partial derivatives of first order (except at the Coulomb-type singular points of the potential) which are *bounded* (see Theorems I, II, Section 2). Actually we are able to describe in more detail 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".<sup>3</sup> 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.

The nature of the singularities of the genuine eigenfunctions of the

---

\*The research reported in this article has been made possible through support and sponsorship extended by the Geophysics Research Directorate, Air Force Cambridge Research Center, under Contract No. AF 19(122)-463.

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

<sup>2</sup>The configuration space is the  $3s$ -dimensional space, the coordinates of which are the coordinates of all  $s$  particles.

<sup>3</sup>For similar use of the word see e.g. Friedrichs [2].

helium atom has been investigated previously (Kemble [3], Gronwall [4], Bartlett [5]). Gronwall discovered a transformation of the helium wave equation into a simple form, and Bartlett continued to work along these lines. But, 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.

Our results stated above show, however, 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 and the 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])

$$(1.1) \quad \phi = e^{-r}, \quad r = (x^2 + y^2 + z^2)^{1/2},$$

in a suitable system of units. Thus  $\phi$  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. We rather 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 use 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 square integrable and bounded at infinity.

The present work was suggested by 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 the 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, at least qualitative, information on the singularities of the eigenfunctions is desirable in choosing good trial functions. 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, where they may well have some sort of singularity. 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 the 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])

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

Here  $\mathbf{r}_i = (x_i, y_i, z_i)$  is the three-dimensional position vector of the  $i$ -th particle, and  $\text{grad}_i$  is the vector operator  $(\partial/\partial x_i, \partial/\partial y_i, \partial/\partial z_i)$ ; the  $\mu_i$  are constants with  $\mu_i > 0$  for  $i = 1, \dots, s$  and  $\mu_0 \geq 0$ . The term with  $\mu_0$  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  $W(\mathbf{r}_1, \dots, \mathbf{r}_s)$  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  $r_i = |\mathbf{r}_i|$ ,  $r_{ij} = |\mathbf{r}_i - \mathbf{r}_j|$ . 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

$$(2.2) \quad W(\mathbf{r}_1, \dots, \mathbf{r}_s) = W_0(\mathbf{r}_1, \dots, \mathbf{r}_s) + \sum_{i=1}^s V_{0i}(\mathbf{r}_i) + \sum_{i < j} V_{ij}(\mathbf{r}_i - \mathbf{r}_j),$$

where

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

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

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

where  $\sigma$  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), 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  $r \leq \varrho$ ,  $\varrho > 0$ , and equal to 0 otherwise. Then the first term on the right-hand side of (2.4) satisfies the condition ii) with any  $\sigma$  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  $V_{ij}(\mathbf{r})$  are *locally square integrable and bounded at infinity*—disappears if we decompose each  $V_{ij}(\mathbf{r})$  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  $\sigma$ , it is *a fortiori* true for smaller  $\sigma > 0$ , since the  $V_{ij}(\mathbf{r})$  are assumed to vanish outside of a sphere. Thus the assumption (2.3) is stronger for larger  $\sigma$ , and we expect to obtain sharper results in this case. This is the reason why we have left  $\sigma$  unspecified.

Before we state the 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; it is these continuity conditions that we shall determine in the present 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 was proved in [1] that there exists a self-adjoint operator  $\tilde{H}$  (in the Hilbert space of square integrable functions

defined in the configuration space) which is uniquely determined by the formal differential operator  $H$  in a natural way. In the proof the potential  $W$  was 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  $\phi$  of this operator  $\tilde{H}$  belonging to a point eigenvalue  $\lambda$ ; thus  $\phi$  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  $\phi$  such that  $\tilde{H}\phi = (E_b - E_a)\phi$  with some  $-\infty < a < b < \infty$ , where  $E_\lambda$  is the resolution of the identity which corresponds 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 be further generalized to include functions belonging to the domain of  $\tilde{H}^n$  for sufficiently large but finite  $n$ , which, however, will not be done here for the sake of simplicity.

It should be noted that  $\tilde{H}$  is not a differential operator in the usual sense; hence 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  $\phi$  (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 mentioned 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  $\phi$  is  $(C_\theta)$  if it is uniformly Hölder continuous with exponent  $\theta$ , that is, if there exist constants  $C$  and  $\theta$ ,  $0 < \theta < 1$ , 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,  $\phi$  is said to be  $(C'_\theta)$  if all first-order partial derivatives of  $\phi$  exist and are  $(C_\theta)$ . It should be noted that we consider only the values  $0 < \theta < 1$ ; thus if we say e.g. that  $\phi$  is  $(C_\theta)$  for

any  $\theta$  with  $\alpha < \theta < \beta$ , this actually implies that  $\phi$  is  $(C_\theta)$  for any  $\theta$  with  $\text{Max}(0, \alpha) < \theta < \text{Min}(1, \beta)$ .

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  $(C_\theta)$  with any  $\theta < 2-3/\sigma$ . If  $\sigma > 3$ , they are  $(C'_\theta)$  with any  $\theta < 1-3/\sigma$ .*

The Coulomb potential corresponds to the case in which  $\sigma$  is smaller than, but may be arbitrarily close to, 3. In this case Theorem I shows that the eigenfunctions are  $(C_\theta)$  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  $0 \leq i < j \leq s$ ,  $V_{ij}(\mathbf{r})$  has the form

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

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

Any point where at least one of the  $r_i$  or  $r_{ij}$  vanishes will be called a Coulomb singular point. Thus Coulomb singular points form  $(3s-3)$ -dimensional hyperplanes, the number of which is  $\frac{1}{2}s(s+1)$ . 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; these derivatives are bounded.*

We can describe in somewhat more detail the nature of the singularities of the eigenfunctions. To do this, we have to introduce a linear transformation of the  $3s$  coordinates  $\mathbf{r}_1, \dots, \mathbf{r}_s$  in order to transform 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 to note, for later use, that our purpose is achieved by a linear transformation of the *special form*

$$(2.6) \quad \mathbf{r}'_i = \sum_{k=1}^s a_{ik} \mathbf{r}_k, \quad i = 1, \dots, s,$$

which transforms each of the three sets of coordinates  $(x_i)$ ,  $(y_i)$ ,  $(z_i)$  into themselves and in the same way. This is obvious from (2.1).<sup>4</sup> We note also that such a linear transformation does not change the square integrability and the properties  $(C_\theta)$ ,  $(C'_\theta)$ , etc., of a function.

<sup>4</sup>An example of such a transformation is given in Kemble [3], pp. 64 and 209.

We denote the new coordinates by  $\mathbf{x} = (x_1, \dots, x_m)$ ,  $m = 3s$ , the new configuration space by  $E_m$ , and the Hilbert space  $L^2(E_m)$  of all square integrable functions by  $\mathfrak{H}$ . The operator (2.1) can now be written as

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

where

$$(2.8) \quad \Delta = \sum_{i=1}^m \frac{\partial^2}{\partial x_i^2},$$

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

the  $V_i(\mathbf{x})$ ,  $i = 1, \dots, M$ ,  $M = \frac{1}{2}s(s+1)$ , correspond to  $V_{0i}(\mathbf{r}_i)$  and  $V_{ij}(\mathbf{r}_i - \mathbf{r}_j)$  of (2.2) in some definite order.

It is now no longer true that each of the  $V_i(\mathbf{x})$  depends only on three coordinates. However, 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, in the new coordinate system  $\tilde{\mathbf{x}} = (\tilde{x}_1, \dots, \tilde{x}_m)$ , the form

$$(2.9) \quad V_i(\mathbf{x}) = \tilde{V}_i(\tilde{x}_1, \tilde{x}_2, \tilde{x}_3).$$

Such an orthogonal transformation leaves the Laplacian  $\Delta$  in (2.7) unchanged. Furthermore, it is clear that the functions  $\tilde{V}_i$  have 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  $\tilde{V}_i(x_1, x_2, x_3)$  vanish outside of a (three-dimensional) sphere and

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

Of course (2.10) is still true if  $\sigma$  is replaced by a smaller positive number. Similarly, if the  $V_{ij}$  satisfy the condition ii'), we can express  $\tilde{V}$  in the form

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

where now  $r = (x_1^2 + x_2^2 + x_3^2)^{1/2}$ ,  $\bar{e}_{ij}$  is a constant,  $\bar{\eta}(r)$  is a function similar to  $\eta(r)$  of (2.4), and the  $\tilde{V}'_i$  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 can be seen without difficulty, will the new  $r$  be *symmetric* 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 corresponding coordinate system 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* and the rest,  $\bar{x}_4, \dots, \bar{x}_m$ , *external* coordinates with respect to  $V_i$ . 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 the trivial example  $V_i = 0$ . But in most cases the distinction is quite clear.

We can now supplement Theorems I and II by

**THEOREM Ia.** *Let, in Theorem I,  $\sigma > 2$ . Then any eigenfunction  $\phi$  is the sum of  $M = \frac{1}{2}s(s+1)$  terms  $\phi_1, \dots, \phi_M$  such that, for each  $i$ ,  $\phi_i$  is  $(C_\theta)$  with any  $\theta < 2-3/\sigma$ , and all external derivatives of  $\phi_i$  with respect to  $V_i$  exist and are  $(C_\theta)$  with any  $\theta < 3-6/\sigma$ .*

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  $\phi_i$ . 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  $\phi$  is the sum of  $M+1$  functions  $\phi_0, \phi_1, \dots, \phi_M$  with the following properties:*

1)  $\phi_0$  is  $(C'_\theta)$  for any  $\theta < 1-3/\sigma$ .

2) If  $x = (x_1, \dots, x_m)$  is a canonical coordinate system for  $V_i$ , then  $\phi_i$  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  $\phi_i$  is  $(C'_\theta)$  in these variables for any  $\theta < 1$ .

That  $\phi_i$  is  $(C'_\theta)$  as a function of  $r, x_4, \dots, x_m$  does not imply that it is  $(C'_\theta)$  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  $\phi$  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 that the internal derivatives of  $\phi$  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 yielding the measure of the discontinuity of  $\partial\phi/\partial x_k$ . As is easily seen from (2.12) it is equal to  $(\partial\bar{\phi}/\partial r)_{r=0}$ , where  $\bar{\phi}$  is the average value of  $\phi$  taken over the sphere  $r = \text{const.}$  for fixed values of  $x_4, \dots, x_m$  (except, of course, for the unimportant case mentioned above).

Now it is interesting to note that this quantity  $(\partial\bar{\phi}/\partial r)_{r=0} = (\partial\phi_i/\partial r)_{r=0}$  is proportional to  $\phi(0, 0, 0, x_4, \dots, x_m)$ . 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*

$$(2.13) \quad \left(\frac{\partial\bar{\phi}}{\partial r}\right)_{r=0} = \frac{1}{2} \bar{e}_i \phi(0, 0, 0, x_4, \dots, x_m)$$

except at some points  $(x_4, \dots, x_m)$  of a set of lower dimension. Here  $\bar{\phi}$  is defined as above and  $\bar{e}_i$  is the constant appearing in the expression (2.11) for  $\bar{V}_i$ .

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 coefficients  $\frac{1}{2}\bar{e}_i$  if the operator is written as

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

This result is not quite trivial even for the hydrogen atom, since  $\phi$  may be any wave packet. Of course it could be verified directly for each eigenfunction.<sup>5</sup>

We shall apply the above results to the case  $s = 2$ . For simplicity we neglect the  $\mu_0$ -term in the Hamiltonian:

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

Then we 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)

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

where  $\bar{\phi}^1$  is the average of  $\phi$  for  $r_1 = \text{const.}$  and  $\bar{\phi}^2$  for  $r_2 = \text{const.}$  To

<sup>5</sup>This result follows also from the ordinary differential equation satisfied by the radial part of the eigenfunction of the hydrogen atom.

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

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

Hence if we write  $\phi(r_1, r_2) = \Psi(\bar{r}_1, \bar{r}_2)$ , we have

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

But

$$\Psi(0, \bar{r}_2) = \phi(2^{-1/2} \bar{r}_2, 2^{-1/2} \bar{r}_2) = \phi\left(\frac{1}{2}(r_1 + r_2), \frac{1}{2}(r_1 + r_2)\right)$$

and

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

so that we get

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

Of course here  $\hat{\phi}^{12}$  means the average of  $\phi$  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  $e_1 = e_2 = -2$ ,  $e_{12} = 0$ . The eigenvalue problem can be solved by separation of variables. The ground state solution is

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

and (2.14) is immediately verified.

A remark is in order here. By Theorem IIa,  $\phi$  should be written as the sum  $\phi = \phi_0 + \phi_1 + \phi_2$ , where  $\phi_0$  is fairly regular and  $\phi_1$  and  $\phi_2$  have singularities with respect to  $r_1$  and  $r_2$ , respectively. But (2.16) shows that  $\phi$  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  $\phi$  can be expressed as a sum of the above form. Nevertheless this should be possible according to the general result and in fact, we can write, for example,

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

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

### 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 a 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 the 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  $\mathfrak{H} = L^2(E_m)$ , 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  $\mathfrak{H}$ :

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

Here and in what follows integrals without any specified region of integration are to be taken over the whole space. Actually the integral in (3.1) is understood in the sense of mean convergence in  $L^2$ . The set of the  $F(p)$  is exactly  $L^2$  over the  $p$ -space, and the correspondence  $f(x) \leftrightarrow F(p)$  is unitary. The functions  $f(x)$  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

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

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

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

It is clear that  $T_0$  thus defined is a self-adjoint operator. Its domain  $\mathfrak{D}_0$  can also be characterized directly in terms of the configuration representation  $f(x)$  with the aid of the notion of the class  $\mathfrak{B}_2^6$ , 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 definite meaning;  $T_0 f$  is also defined for such  $f$  and we 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  $f \in \mathfrak{D}_0$ , there is a sequence  $\{f_n\}$  of smooth functions of the above kind<sup>7</sup> 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  $\mathfrak{H}$ .

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  $\mathfrak{H}$  is clear:  $Wf$  is defined if and only if  $f$  and  $Wf$  are square integrable.

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

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

This implies that  $\tilde{H}$  has the same domain  $\mathfrak{D}_0$  as  $T_0$  and  $\tilde{H}f = T_0 f + Wf$  for  $f \in \mathfrak{D}_0$ . 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  $\mathfrak{D}_0$ , 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

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

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

Prescribing 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  $E_m$ .

<sup>6</sup>See Calkin [10] and Morrey [11].

<sup>7</sup>It has been proved in [1] that  $f_n$  may be assumed to have the form  $P(x)e^{-x^2/2}$ , where  $P(x)$  is a polynomial of  $x_1, \dots, x_m$ .

The function  $g(x)$  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  $m$ -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) yields

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

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  $\mathfrak{D}_0$ . To do this we note that  $G$  and  $K$  are bounded linear operators defined everywhere in  $\mathfrak{H}$ . This follows from the fact that the functions  $g(x)$  and  $k(x)$  are integrable in the whole space<sup>a</sup>.

Now let  $u \in \mathfrak{D}_0$  be arbitrary. Then there exists 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 for  $n \rightarrow \infty$  gives the desired result (3.10) for any  $u \in \mathfrak{D}_0$ .

We know that  $\tilde{H}u$  is defined for any  $u \in \mathfrak{D}_0$  and that  $\tilde{H}u = T_0 u + Wu$ , i.e., that  $T_0 u = \tilde{H}u - Wu$ . Inserting this into (3.10), we obtain

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

<sup>a</sup>For completeness we sketch a proof here. We have for any  $u \in \mathfrak{H}$

$$\left[ \int |g(x-y)| |u(y)| dy \right]^2 \leq \int |g(x-y)|^2 dy \int |u(y)|^2 dy = C \int |g(x-y)| |u(y)|^2 dy,$$

where we set  $C = \int |g(x)| dx$ . Hence

$$\int dx \left[ \int |g(x-y)| |u(y)|^2 dy \right] \leq C \int |u(y)|^2 dy \int |g(x-y)| dx = C^2 \|u\|^2.$$

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

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

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

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

#### 4. Lemmas on 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  $\mathfrak{S}$ , as shown in the preceding section. In particular, since the kernel  $k(x-y)$  of  $K$  is a smooth function,  $K$  transforms every function  $u \in \mathfrak{S}$  into a smooth function. The kernel  $g(x-y)$  of  $G$  has a singularity given by (3.7), but this singularity is familiar from 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. 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  $u$  for which both the  $V_i u$  and the  $G(V_i u)$  are 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, for simplicity,  $V$  stand for any one of the  $V_i$ . Then the operator  $GV$  is obviously a restriction on 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  $\mathfrak{S}$ .

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,  $\|u\|_\infty = \sup |u(x)|$ . If we consider  $A$  as a linear operator on functions in  $L^p$  to functions in  $L^q$ ,  $Au$  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 denote it by  $A_p^q$ .

Similarly we shall consider the operator  $B = GW_0$  for which

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

in the same Banach spaces, and use the notation  $B_p^q$ .

For these operators, we now prove several lemmas. Here we assume that  $V(x) = V_i(x)$  is of the general form (2.9) satisfying (2.10). We begin with the auxiliary

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  $\alpha, \beta$  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<sup>9</sup>

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

Proof: First we note the simple formula

$$(4.6) \quad \int |x|^{-\nu}\zeta_1(|x|)dx_4 \cdots dx_m = \frac{\pi^{(m-3)/2} \Gamma\left(\frac{\nu-m+3}{2}\right)}{\Gamma\left(\frac{\nu}{2}\right)} r^{-\nu+m-3} + f(r^2),$$

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  $\lambda = (x_4^2 + \cdots + x_m^2)^{1/2}$  and transform the integral into

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

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  $V = \bar{V}(x_1, x_2, x_3)$  (see (2.9)). This does not affect the generality; for, an orthogonal transformation

<sup>9</sup>If  $\alpha = 0$ ,  $|g_\mu(x-y)|^\alpha$  in (4.5) is to be set equal to zero whenever  $g_\mu(x-y) = 0$ . In other words, the integral in (4.5) is a finite integral taken over  $|y-x| \leq 2$  whether or not  $\alpha > 0$ .

of the coordinates  $x_1, \dots, x_m$  does not change the form of  $g_\mu$ . Then, denoting the integral (4.5) by  $I(x)$ , we have

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

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  $C s^{-\alpha(m-\mu)+m-3}$  with some constant  $C$ . Thus we have

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

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 because of (4.8) and because we have assumed  $\beta > 0$ . 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 Hölder's inequality to the integral on the right-hand side of (4.9), we obtain

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

The second factor is finite and independent of  $x$ , since  $[\alpha(m-\mu) - (m-3)]a < 3$  by (4.10). The first factor is not decreased if the region of integration is replaced 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  $\alpha', \beta$  instead of  $\alpha, \beta$ . Furthermore  $\alpha'(m-\mu) > m-3$ , and thus (4.8) is also satisfied by  $\alpha'$ . Therefore, (4.5) is seen to hold if  $\alpha$  is replaced by  $\alpha'$ . Also<sup>10</sup>, (4.5) is true for  $\alpha = 0$ , if  $0 < \beta < \sigma$ . Hence (4.5) must hold for any  $\alpha$  between 0 and  $\alpha'$ , and in particular for our  $\alpha$ , 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,  $\int |g_\mu(y)|^\alpha dy_4 \cdots dy_m$ , of (4.7) has an upper bound independent of  $(y_1, y_2, y_3)$ <sup>11</sup> and 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  $1/q > 1/p - 2/m$ , then  $B_p^q$  is a bounded linear operator defined everywhere in  $L^p$ . If

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

then the same is true for  $A_p^q$ .

Proof: We first give the proof for  $A_p^q$ . Let  $m_0 = \text{Min} [m, (2-3/\sigma)p]$  and let  $\varepsilon$  be such that  $0 < \varepsilon < \frac{1}{2}m_0$ . Furthermore, set

$$\begin{aligned} \gamma &= \frac{m-\varepsilon}{m-2}, & \delta &= \frac{m_0-2\varepsilon}{m-2}, & \alpha &= \frac{p-\gamma+\delta}{p-1}, \\ \beta &= \frac{p}{p-1}, & q &= \frac{\gamma p}{\gamma-\delta}. \end{aligned}$$

Since  $m \geq m_0$  and  $0 < \varepsilon < \frac{1}{2}m_0$ , we see that  $\gamma > \delta > 0$  and hence  $q > p$ . Also  $\beta > 0$  and  $\gamma < m/(m-2) \leq 2 \leq p$ , so that  $\alpha > 0$ . Moreover, it is easily seen that

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

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

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

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

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

<sup>10</sup>See footnote 9.

<sup>11</sup>Again see footnote 9.

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

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

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

It is easy to verify that

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

therefore,

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

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 with  $\beta = p(p-1)^{-1} \leq 2 \leq \sigma$ . 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<sup>12</sup>

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

i.e. at

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

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, by a suitable choice of  $\varepsilon$ ,  $0 < \varepsilon < \frac{1}{2}m_0$ ,  $q$  can be made to satisfy  $p < q < mp(m-m_0)^{-1}$ . In other words,  $q$  may be arbitrary if

<sup>12</sup>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  $q = \infty$ . The case  $q = p < \infty$  is obtained if we use  $\varepsilon = \frac{1}{2}m_0$  in our 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  $p > m(2-3/\sigma)^{-1}$ , then the function  $Au$  is bounded and  $(C_\theta)$  for any  $\theta < 2-3/\sigma-m/p$ . If  $u \in L^p$  with  $p > \frac{1}{2}m$ , then  $Bu$  is bounded and  $(C_\theta)$  for any  $\theta < 2-m/p$  ( $p \geq 2$  is always assumed).*

Proof: First we prove

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

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

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,

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

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

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

where  $\text{Max}_{\tau \geq t} |\zeta'(\tau)|$  is a function equal to a constant for  $t \leq 1$  and vanishing for  $t \geq 2$ . We can, therefore, write  $\text{Max}_{\tau \geq t} |\zeta'(\tau)|$  as  $C\zeta_2(t)$ , where the function  $\zeta_2(t)$  has the property (3.6).

Collecting the above results, we obtain

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

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

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

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  $A_p^\infty$  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

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

with  $\beta = p/(p-1) \leq \sigma$ . Here

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

if  $\theta < 2-3/\sigma-m/p$ . 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  $\beta$  has only to satisfy  $\beta < m(m-\mu)^{-1}$ , and this is the case if  $\theta < 2-m/p$ .

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

*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  $(C_\theta)$ , the formal differentiation is easily justified and the lemma is proved. But the continuity of (4.17) can be shown 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  $(C_\delta)$  with some  $\delta > 3/\sigma - 1$ . Then  $Au$  has external partial derivatives with respect to  $V$ , which are  $(C_\theta)$  for any  $\theta < \delta + 1 - 3/\sigma$ .*

*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 the external coordinates  $x_i$ ,  $i = 4, \dots, m$ , which can be written as

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

since the integral involving  $u(x)$  vanishes, because of symmetry. By hypothesis,  $|u(y) - u(x)| \leq C |y-x|^\delta$ , therefore the integrand in (4.20) is majorized by  $C |g_0(x-y)| |x-y|^{1+\delta} |\bar{V}(y_1, y_2, y_3)|$  which, in the notation of Lemma 1, is of the form  $C |g_{1+\delta}(x-y)| |V(y)|$ . Applying Lemma 1 with  $\alpha = \beta = 1$ , we see that the integral (4.20) has a finite upper bound independent of  $x$  and thus is absolutely convergent.

If we can show the Hölder continuity of the function 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 well-known procedure, we take a sphere  $\Sigma$  with center  $x$  and radius  $2|x' - x| = \varrho$ , and write

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

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 method we used to show that  $v(x)$  exists, the only difference being in the region of integration. Inspecting the proof of Lemma 1, it is easily seen that

$$|I_1| \leq C \left[ \int_{s \leq \varrho} s^{-(2-\delta)\alpha} \cdot 4\pi s^2 ds \right]^{1/\alpha} \leq C \varrho^{3/\alpha - (2-\delta)},$$

where, by (4.10),

$$\frac{1}{\alpha} = 1 - \frac{1}{b} = 1 - \frac{1}{\sigma}$$

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

To get an estimate for  $I_3$  we use (4.19):

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

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 have

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

In particular, let  $\theta$  be such that  $\theta < \delta + 1 - 3/\sigma$ . Then  $1 - \theta + \delta > 3/\sigma$  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 collecting our results, we see that  $|v(x') - v(x)| \leq C \varrho^\theta = C |x' - x|^\theta$  if  $\theta < 1$ ,  $\theta < \delta + 1 - 3/\sigma$  and  $|x' - x|$  is bounded. But the last restriction for  $|x' - x|$  is not necessary, since  $v(x)$  is bounded. This completes the proof of Lemma 5.

## 5. Proof of Theorems I and Ia

We first prove

LEMMA 6. Let  $u \in \mathfrak{D}_0$  and  $\tilde{H}u \in L^p$  for some  $p \geq 2$ . Then  $u \in L^q$  for any  $q \geq 0$  such that  $\frac{1}{2} \geq 1/q > 1/p - 2/m$ . If  $p > \frac{1}{2}m$ , then  $u$  is bounded and

$(C_\theta)$  for any  $\theta < \min(2-m/p, 2-3/\sigma)$ . Furthermore, if  $p > m$  and  $\sigma > 3$ ,  $u$  is  $(C'_\theta)$  for any  $\theta < \min(1-m/p, 1-3/\sigma)$ .

Proof: Let  $J$  be the set of positive numbers  $q$  (including  $\infty$ ) such that  $u \in L^q$ . Since  $u \in \mathfrak{H} = L^2$ ,  $J$  contains at least one point, i.e.  $q = 2$ . As is well known,  $J$  is an interval. Let  $b$  be the right end point of this interval. Then, for any  $\varepsilon > 0$ , there is a number  $q' \in J$  such that  $1/q' < 1/b + \varepsilon$ .

The integral expression (3.11) can be written as

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

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  $\mathfrak{H} = L^2$ .

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  $1/p \geq 1/q > 1/p - 2/m$ , as seen from Lemma 2.<sup>13</sup> But since  $G\tilde{H}u \in L^2$ , this is true with any  $q$  such that  $\frac{1}{2} \geq 1/q > 1/p - 2/m$ . For the same reason, the third term of (5.1),  $-Bu$ , belongs to  $L^q$  with any  $q$  such that  $\frac{1}{2} \geq 1/q > 1/q' - 2/m$ , for  $u \in L^{q'}$ . Similarly by Lemma 2, it follows that each  $A_i u \in L^q$  with any  $q$  such that  $\frac{1}{2} \geq 1/q > 1/q' - (2-3/\sigma)/m$ . 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  $1/q$  is larger than the largest number among  $0, 1/p - 2/m, 1/q' - 2/m, 1/q' - (2-3/\sigma)/m$ . Noting that the fourth of these expressions is larger than the third, we see that

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

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

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

This proves the first part of Lemma 6.

Next suppose that  $p > \frac{1}{2}m$ . 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  $(C_\theta)$  for any  $\theta < 2-3/\sigma$  and that  $Bu$  is  $(C_\theta)$  for any  $\theta < 2$  (in fact, for  $\theta < 1$ ). Since

<sup>13</sup>In Lemma 2 we assumed  $m \geq 4$ , hence, the argument here is not applicable to the case  $m = 3$ . However, we know (see [1]) that every  $u \in \mathfrak{D}_0$  is continuous and bounded if  $m = 3$ . Thus Lemma 6 holds for all  $m \geq 3$ .

$\tilde{H}u \in L^p$ , Lemma 3 with  $G = B$  also shows that  $G\tilde{H}u$  is  $(C_\theta)$  for any  $\theta < 2 - m/p$ . Finally  $Ku$  is a smooth function and hence is  $(C_\theta)$  for any  $\theta < 1$ . Summing up, we conclude that  $u$  is  $(C_\theta)$  with any  $\theta < \min(2 - 3/\sigma, 2 - m/p)$ . This proves the second part of Lemma 6.

The last part follows 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  $f_1 \in \mathfrak{D}_0$  and  $\tilde{H}f_1 = f_0 \in \mathfrak{S} = L^2$ , Lemma 6 implies that  $f_1 \in L^q$  for any  $1/q > \frac{1}{2} - 2/m$ . Since in turn  $\tilde{H}f_2 = f_1$ , it follows from Lemma 6 that  $f_2 \in L^q$  for any  $1/q > \frac{1}{2} - 4/m$ . Repeating this argument, we see that  $f_k \in L^q$  for any  $1/q > \frac{1}{2} - 2k/m$ . If we take  $k$  equal to the first integer larger than  $m/4 - \frac{1}{2}$ , we have  $f_k \in L^q$  with some  $q > m$ . Then, by Lemma 6,  $f_{k+1}$  must be  $(C_\theta)$  for any  $\theta < 2 - 3/\sigma$ . 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  $(C_\theta)$  with any  $\theta < 2 - 3/\sigma$ . 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  $\theta < 1 - 3/\sigma$ , and the second part of Theorem I follows as above.

Theorem Ia can be proved by making use of Lemma 5. Let  $\phi$  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  $(C_\theta)$  with some  $\theta$ , 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  $(C'_\theta)$  for any  $\theta < 1$ , by Lemma 4. Thus the sum of the first three terms of (5.2) is  $(C'_\theta)$  for any  $\theta < 1$ .

Let  $\phi_i = -A_i\phi$ . We know by Theorem I that  $\phi \in (C_\delta)$  for any  $\delta < 2 - 3/\sigma$ . Noting that  $2 - 3/\sigma > 3/\sigma - 1$  by the assumption  $\sigma > 2$ , we see from Lemma 5 that  $\phi_i$  has external derivatives which are  $(C_\theta)$  with any  $\theta < 2 - 3/\sigma + 1 - 3/\sigma = 3 - 6/\sigma$ . This proves Theorem Ia since the first three terms of (5.2) may be added to any of the  $\phi_i$  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  $V$  anyone 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,

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

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  $(C_\delta)$  for some  $\delta > 1 - 3/m$ . Then  $Au$  can be written as  $Au = v + w$ , where  $v$  and  $w$  have the following properties:  $v$  is  $(C'_\theta)$  for any  $\theta < \min[1 - 3/\sigma, 1 - (1 - \delta)m/3]$ ,  $w$  is a function of  $r$  and of the external coordinates  $x_4, \dots, x_m$  only,  $w \in (C'_\theta)$  for any  $\theta < \delta$  in the variables  $r, x_4, \dots, x_m$ , and

$$(6.3) \quad \left( \frac{\partial w}{\partial r} \right)_{r=0} = -\frac{1}{2} \bar{e} u(0, 0, 0, x_4, \dots, x_m).$$

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  $(C'_\theta)$  for any  $\theta < 1 - 3/\sigma$ ; this follows from Lemma 4, where we may let  $p \rightarrow \infty$ . Thus this contribution satisfies the condition on  $v$  stated in Lemma 7. In what follows we may, therefore, assume

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

Here  $\bar{\eta}(r) = 1$  for  $r \leq \varrho$  and  $\bar{\eta}(r) = 0$  for  $r > \varrho$  with some constant  $\varrho > 0$  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

$$(6.6) \quad u_0(x) = u(0, 0, 0, x_4, \dots, x_m).$$

Then the contribution to  $Au$  from the second term of (6.5) is seen to be Hölder continuous. In fact, since, by hypothesis,  $|u(x) - u_0(x)| \leq Cr^\delta$  and since (6.4) is true, the function  $z(x) = V(x)[u(x) - u_0(x)]$  belongs to  $L^p$  at least locally (and uniformly)<sup>14</sup>, with any  $p$  such that  $(1 - \delta)p < 3$ . Lemma 4<sup>15</sup> applied to  $Bz$  with  $B = G$  implies that this contribution  $Gz$  is  $(C'_\theta)$  for

<sup>14</sup>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.

<sup>15</sup>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  $|y - x| \leq 2$ .

any  $\theta < 1 - m/p$  and hence any  $\theta < 1 - (1 - \delta)m/3$ . 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 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  $w_{x_i}(x)$ ,  $i \geq 4$ , are  $(C_\theta)$  with any  $\theta < \delta$ , because, for the Coulomb potential (6.4), we may take  $\sigma$  arbitrarily close to 3.

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),

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

this is certainly true if  $x_1 > 0$ , and then represents a function which is smooth. 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  $(C_\theta)$  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 three-dimensional integral by (4.6), since 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 in (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  $s = (y_1^2 + y_2^2 + y_3^2)^{1/2}$ ,  $t = [(x_1 - y_1)^2 + y_2^2 + y_3^2]^{1/2}$ , and  $f(t^2)$  is a smooth function of  $t^2$ , at least for  $t^2 < 1$ . The second integral in (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  $\rho$ ). 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 the dots stand for a function which is at least  $(C_\theta)$  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  $\phi$  are bounded and  $(C_\theta)$  for any  $\theta < 1$ . Then we consider the integral expression (5.2). Since  $\tilde{H}\phi$  as well as  $\phi$  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  $\delta$  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  $\Psi_i$  is  $(C'_\theta)$  for any  $\theta < 1 - 3/\sigma$  and  $\phi_i$  is a function  $(C'_\theta)$  for any  $\theta < 1$  of  $m-2$  variables, which are  $r, x_4, \dots, x_m$  in the canonical coordinate system for the  $V_i$ . If we combine all the  $\Psi_i$  together with the smooth function given by the first three terms of (5.2) into one function  $\phi_0$ , the assertion of Theorem IIa is proved. Theorem IIb then follows from (6.3) and the discussion given after the statement of Theorem IIa.

### Bibliography

- [1] Kato, T., *Fundamental properties of Hamiltonian operators of Schrödinger type*, Trans. Amer. Math. Soc., Vol. 70, 1951, pp. 195-211.
- [2] Friedrichs, K. O., *On differential operators in Hilbert spaces*, Amer. J. Math., Vol. 61, 1939, pp. 523-544.
- [3] Kemble, E. C., *The Fundamental Principles of Quantum Mechanics*, International Series in Physics, McGraw-Hill, New York and London, 1937.
- [4] Gronwall, T. H., *Helium wave equation*, Physical Rev., Vol. 51, 1937, pp. 655-660.
- [5] Bartlett, J. H., Jr., *Helium wave equation*, Physical Rev., Vol. 51, 1937, pp. 661-669.
- [6] Chandrasekhar, S., and Herzberg, G., *Energies of the ground states of He, Li<sup>+</sup> and O<sup>++</sup>*, Physical Rev., Vol. 98, 1955, pp. 1050-1054.
- [7] Kinoshita, T., *The ground state of the helium atom*, to be published.
- [8] Hylleraas, E. A., *Neue Berechnung der Energie des Heliums im Grundzustande, sowie des tiefsten Terms von Ortho-Helium*, Z. Physik, Vol. 54, 1929, pp. 347-366. *Ueber den Grundterm der Zweielektronenprobleme von H<sup>-</sup>, He, Li<sup>+</sup>, Be<sup>++</sup> usw.*, Z. Physik, Vol. 65, 1930, pp. 209-225.
- [9] von Neumann, J., *Mathematische Grundlagen der Quantenmechanik*, Springer, Berlin, 1932.
- [10] Calkin, J. W., *Functions of several variables and absolute continuity, I*, Duke Math. J., Vol. 6, 1940, pp. 170-186.
- [11] Morrey, C. B., Jr., *Functions of several variables and absolute continuity, II*, Duke Math. J., Vol. 6, 1940, pp. 187-215.

Received June, 1956.