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Error and Convergence Bounds for the Born Expansion

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For scattering in nonrelativistic quantum mechanics, the range of validity of the perturbation expansion is studied by viewing the expansion as being generated by an iteration procedure, and applying to it a fundamental theorem for iteration processes. The theorem provides a sufficient condition for convergence and, at the same time, gives upper bounds on the error generated in truncating the expansion at a given number of terms. These error bounds for the wave function are in turn used to find upper bounds on the truncation error for the S-matrix expansion. Bounds for the exact S matrix are also given. These results are illustrated by applying them to the simple case of one-particle potential scattering, for both the plane-wave and partial-wave analyses.

I. INTRODUCTION

GIVEN a system with Hamiltonian $H=H_0+\lambda V$, one of the most generally applied methods of solving for its quantum scattering states is the Born perturbation expansion,[1] which expresses the wave function as a power series in λ. In examining the range of validity of this method—that is, the radius of the circle of convergence in the λ plane—there have been applied to date two major approaches:

(1) Bounds on the radius of convergence are obtained by comparing, term for term, the Born expansion with another power series known to converge, and

(2) One studies the determinantal solution

$$\psi=\phi+\lambda(D\phi/d), \tag{1.1}$$

where ψ and ϕ are the scattering and free wave functions, and the operator D and number d are expressed as power series in λ. These power series always converge for non-pathological cases; hence the radius of convergence of the Born series is $|\lambda_c|$, where λ_c is the smallest zero[2] of $d(\lambda)$.

In this paper another major approach is developed, which will turn out to be a variant of (1) above. The Born expansion is viewed as being generated by an iterative process, and we make a simple, straightforward application of a fundamental theorem for iteration procedures. This theorem (for our purposes we shall call it the Banach-Weissinger theorem[3]) has been curiously ignored by physicists; for convenience it is presented in Appendix 1. The theorem immediately provides a sufficient condition for convergence equivalent to a lower bound on the radius of convergence of the Born series.

In addition to the question of its domain of validity, a subject of considerable interest is the error involved in truncating the Born series after a given number of terms. Despite its importance for numerical calculations, studies in this area have been sparse.[4] In addition to providing a simple, transparent starting point for investigating the convergence of the Born expansion, the Banach-Weissinger theorem automatically yields upper bounds for the truncation error.

The core of this paper is the next section where the above program is effected for the general case of N-particle, nonrelativistic quantum scattering. The results are also used to obtain bounds for the T matrix. We then go on to illustrate these results by applying them to the simple case of one-particle potential scattering. Section III deals with plane-wave scattering; partial-wave scattering is treated in Sec. IV.

II. THE BORN EXPANSION AS AN ITERATION PROCEDURE

Henceforth, we shall consider the coupling constant λ of the previous section to be incorporated into V and not explicitly displayed. $\psi(x)$ shall represent a continuous but otherwise arbitrary function of $x=(x_1,x_2,\cdots,x_N)$; we shall reserve the symbols ψ_0 and ψ_∞ for eigenfunctions of the unperturbed and full Hamiltonians:

$$H_0\psi_0=E\psi_0,$$

and

$$H\psi_\infty=E\psi_\infty.$$

Define the functional F as

$$F(\psi)=\psi_0+GV\psi \equiv\psi_0+\int G(x,x')V(x')\psi(x')dx', \tag{2.1}$$

where

$$G=(E-H_0+i\epsilon)^{-1}.$$

Then the Born expansion[1,5] is generated by the sequence $\psi_0, \psi_1, \psi_2, \cdots$, where

$$\psi_{n+1}=F(\psi_n). \tag{2.2}$$

[1] See for example M. L. Goldberger and K. M. Watson, *Collision Theory* (John Wiley & Sons, Inc., New York, 1964); or T. Y. Wu and T. Ohmura, *Quantum Theory of Scattering* (Prentice-Hall, Inc., Englewood Cliffs, New Jersey, 1962).

[2] In this connection see I. Manning, J. Math. Phys. **5**, 1223 (1964), which relates $d(\lambda)$ to the behavior of ψ at the origin.

[3] The theorem was apparently discovered by S. Banach, Fundamental Math. (Warsaw) **3**, 160 (1922), and independently rediscovered by J. Weissinger, Z. Angew. Math. Mech. **31**, 245 (1951) and Math. Nachr. **8**, 193 (1952). In the Russian literature one frequently finds it referred to as the contraction mapping principle. See for example V. V. Nemitsky, Uspekhi Mat. Nauk. **1**, 141 (1936) [Amer. Math. Soc. Translations, Ser. 2, **34**, 1 (1963)].

[4] T. Y. Wu and T. Ohmura (Ref. 1), Sec. C.4.

[5] M. Gell-Mann and M. L. Goldberger, Phys. Rev. **91**, 398 (1953).

Let $W(x)$ be a fixed, continuous, positive, finite, but otherwise arbitrary function. We shall use the norm[6]

$$\|\psi\| = \max_x(|\psi(x)|/W(x)). \tag{2.3}$$

Note that

$$\|GV\psi\| \leq \alpha\|\psi\| \tag{2.4}$$

with

$$\alpha = \max_x \frac{1}{W(x)}\int |G(x,x')V(x')|W(x')dx', \tag{2.5}$$

which implies that Eq. (A1.5) of Appendix 1 is satisfied.

The Banach-Weissinger theorem now tells us that a sufficient condition for the convergence of the Born expansion is

$$\alpha < 1, \tag{2.6}$$

in which case the sequence $\{\psi_n\}$ converges to the wave function ψ_∞ satisfying the Lippman-Schwinger equation[7,5]

$$\psi_\infty = F(\psi_\infty). \tag{2.7}$$

We also have the truncation-error bounds

$$\|\psi_\infty - \psi_n\| \leq \alpha(1-\alpha)^{-1}\|\psi_n - \psi_{n-1}\| \tag{2.8}$$

$$\leq \alpha^n(1-\alpha)^{-1}\|\psi_1 - \psi_0\| \tag{2.9}$$

$$\leq \alpha^{n+1}(1-\alpha)^{-1}\|\psi_0\|. \tag{2.10}$$

These bounds can be used to obtain bounds on the truncation error for the S matrix: Write

$$T_{n+1} \equiv \int \psi_0(x)V(x)\psi_n(x)dx, \tag{2.11}$$

so that the T matrix for the scattering problem is T_∞. Also put

$$\beta \equiv \int W^2(x)|V(x)|dx. \tag{2.12}$$

The above bounds then yield

$$|T_\infty - T_{n+1}| \leq \beta\|\psi_0\|\cdot\|\psi_\infty - \psi_n\|$$
$$\leq \beta\alpha(1-\alpha)^{-1}\|\psi_n - \psi_{n-1}\|\cdot\|\psi_0\| \tag{2.13}$$

$$\leq \beta\alpha^n(1-\alpha)^{-1}\|\psi_1 - \psi_0\|\cdot\|\psi_0\| \tag{2.14}$$

$$\leq \beta\alpha^{n+1}(1-\alpha)^{-1}\|\psi_0\|^2. \tag{2.15}$$

The above takes the approach of aiming at bounding the error in an approximate calculation. One can also aim at finding bounds for T_∞ itself. In fact, by calculating or otherwise bounding T_{n+1}, one can use the above expressions to bracket T_∞ with arbitrary precision.[8]

[6] L. Collatz, Z. Angew. Math. Phys. **4**, 327 (1953).
[7] B. A. Lippmann and J. Schwinger, Phys. Rev. **79**, 469 (1950).
[8] In this connection see L. Spruch, *Lectures in Theoretical Physics* (Interscience Publishers, Inc., New York, 1962), Vol. IV, p. 161.

Using $n=0$ as a simple example, we have

$$T_1 = \int \psi_0(x)V(x)\psi_0(x)dx,$$

so

$$|T_1| \leq \beta\|\psi_0\|^2. \tag{2.16}$$

Substituting this bound and Eq. (2.15) into the inequality

$$|T_\infty| \leq |T_1| + |T_\infty - T_1|,$$

we get

$$|T_\infty| \leq \beta(1-\alpha)^{-1}\|\psi_0\|^2. \tag{2.17}$$

The T-matrix bounds require that β exist; with this understanding, all of the above bounds are valid whenever $\alpha < 1$.

III. PLANE-WAVE POTENTIAL SCATTERING

For one-particle plane-wave potential scattering the Green's function is[1] (we use units such that $\hbar = m = 1$; $E = \frac{1}{2}k^2$)

$$G(\mathbf{r},\mathbf{r}') = -\frac{\exp(ik|\mathbf{r}-\mathbf{r}'|)}{2\pi|\mathbf{r}-\mathbf{r}'|}, \tag{3.1}$$

and Eq. (2.5) becomes

$$\alpha = \max_{\mathbf{r}} \frac{1}{2\pi W(\mathbf{r})}\int \frac{|V(\mathbf{r}')|}{|\mathbf{r}-\mathbf{r}'|}W(\mathbf{r}')d^3\mathbf{r}'. \tag{3.2}$$

For $W=1$, the convergence condition $\alpha < \frac{1}{2}$ has been found by Zemach and Klein.[9] In addition to a simplified derivation, we have the improvement of Eq. (2.6). For the remainder of this paper we shall be most often concerned with bounding the quantity α of Eq. (2.5). It should be kept in mind that once $W(x)$ has been fixed and the corresponding α determined, we automatically have all the bounds of Eqs. (2.8) to (2.10), (2.13) to (2.15), and (2.17).

Let

$$\mathbf{V}(r) \equiv \max_{\vartheta,\varphi}|V(r,\vartheta,\varphi)|. \tag{3.3}$$

Then for $W=1$ we have $\alpha \leq \alpha^{(1)}$, with

$$\alpha^{(1)} = 2\int_0^\infty \mathbf{V}(r)rdr. \tag{3.4}$$

IV. PARTIAL-WAVE POTENTIAL SCATTERING

1. General Formulation

For simplicity, consider the potential to be spherically symmetric. [The extension to the more general case is straightforward or, at the expense of obtaining cruder bounds, one may use the $\mathbf{V}(r)$ of the previous section.] For a given partial wave, the wave function may be written

$$\psi_\infty(\mathbf{r}) = (u_\infty(r)/r)Y_{lm}(\hat{r}), \tag{4.1}$$

[9] Ch. Zemach and A. Klein, Nuovo Cimento **10**, 1078 (1958).

and the Born expansion in this case can be represented[1] by a sequence of functions $u_0, u_1, u_2, \cdots$ converging to u_∞:

$$u_{n+1}=F(u_n)\,, \tag{4.2}$$

with

$$F(u)=f(r)+\int_0^\infty G(r,r')V(r')u(r')dr'\,, \tag{4.3}$$

where

$$G(rr')=-i\pi f(r_<)g(r_>)\,, \tag{4.4}$$

$$f(r)=(2k/\pi)^{1/2}rj_l(kr)\,, \tag{4.5}$$

$$g(r)=(2k/\pi)^{1/2}rh_l^{(1)}(kr)\,, \tag{4.6}$$

and

$$u_0=f(r)\,. \tag{4.7}$$

In the above $r_<$ and $r_>$ are, respectively, the lesser and greater of r and r', j_l is the spherical Bessel function,[1] and $h_l^{(1)}$ is the spherical Hankel function of the first kind. We also have

$$T_n=\int_0^\infty f(r)V(r)u_{n-1}(r)dr\,, \tag{4.8}$$

and

$$T_\infty=-\pi^{-1}\sin\delta\,. \tag{4.9}$$

With the norm

$$\|u\|=\max_r(|u(r)|/W(r))\,, \tag{4.10}$$

one finds

$$\|GVu\|\leq\alpha\|u\| \tag{4.11}$$

with

$$\alpha=\max_r\frac{2kr}{W(r)}\times\int_0^\infty r'|j_l(kr_<)h_l^{(1)}(kr_>)V(r')|W(r')dr'\,, \tag{4.12}$$

and all of the corresponding results of Sec. II apply here as well.

We will find it of interest to explore the particular case

$$W=r^\nu. \tag{4.13}$$

Introducing the quantity (further discussed in Appendix 2)

$$b_l(\nu)=\max_x(|j_l(x)|/x^{\nu-1})\,, \tag{4.14}$$

one finds [with the $W(r)$ above]

$$\|f\|=(2/\pi)^{1/2}b_l(\nu)k^{\nu-1/2}. \tag{4.15}$$

The quantity $b_l(\nu)$ will exist as a finite number only if

$$0\leq\nu\leq l+1\,, \tag{4.16}$$

and we therefore shall restrict ourselves to this range for ν. With the substitution of u_n for ψ_n, the various bounds of Sec. II have an obvious transliteration to the present case; for example Eq. (2.17) becomes

$$|T_\infty|\leq 2\pi^{-1}b_l^2(\nu)\beta_\nu(1-\alpha)^{-1}k^{2\nu-1}\,, \tag{4.17}$$

where

$$\beta_\nu=\int r^{2\nu}|V(r)|dr\,. \tag{4.18}$$

Examining the above expression for α, one obtains a useful bound by noting that $\alpha\leq\alpha^{(2)}$ with

$$\alpha^{(2)}=\max_r 2k\left[r^{-\nu+1}|h_l^{(1)}(kr)|\int_0^r r'^{\nu+1}|j_l(kr')V(r')|dr' + k^{\nu-1}b_l(\nu)\int_r^\infty r'^{\nu+1}|h_l^{(1)}(kr')V(r')|dr'\right].$$

If the requirements listed below are met, the derivative with respect to r of the above bracket is always negative[10]; this function therefore achieves its maximum at $r=0$, yielding

$$\alpha^{(2)}=2k^\nu b_l(\nu)\int_0^\infty r'^{\nu+1}|h_l^{(1)}(kr')V(r')|dr'\,, \tag{4.19}$$

providing that

$$0\leq\nu\leq l+1 \quad\text{and}\quad \lim_{r\to0}r^2V(r)=0.$$

2. Bounds Useful at All Energies

Using the formulas of the previous paragraph for α, β, and $\|f\|$, set $\nu=\frac{1}{2}$; the bounds thus generated by the expressions of Sec. II are ones useful at all energies.

In addition to $\alpha^{(2)}$ of the previous paragraph, we obtain another bound on α by defining the quantity

$$a_l\equiv\max_{x,x'}(xx')^{1/2}|j_l(x_<)h_l^{(1)}(x_>)|\,, \tag{4.20}$$

which is further discussed in Appendix 2. Equation (4.12) yields

$$\alpha\leq\alpha^{(3)}\,,$$

where $\nu=\frac{1}{2}$ and

$$\alpha^{(3)}=2a_l\beta_{1/2}. \tag{4.21}$$

The fact that $\alpha^{(3)}<1$ implies convergence of the Born series was found by Kohn, Eq. (11.14) of his work.[11] The truncation-error bound given by our Eq. (2.15)

[10] $x|h_l^{(1)}(x)|$ is a monotonically decreasing function of x, as can be seen from the representation

$$x^2|h_l^{(1)}(x)|^2=\sum_{k=0}^{l}\frac{(2l-k)!(2l-2k)!}{k![(l-k)!]^2}(2x)^{2k-2l}.$$

[*Handbook of Mathematical Functions*, edited by M. Abramowitz and I. A. Stegun (National Bureau of Standards Applied Math. Series No. 55, U. S. Government Printing Office, Washington, D. C., 1964)].

[11] W. Kohn, Rev. Mod. Phys. **26**, 292 (1954).

with $\alpha=\alpha^{(3)}$ was found by Kohn (Ref. 11), in his Eq. (12.2).

We note from Appendix 2 that $a_l \to 0$ as $l \to \infty$; hence, for $\beta_{1/2}$ finite, $\alpha \to 0$ and not only does the Born expansion always converge for l sufficiently large, but $u_\infty \to u_1$ (and $u_1 \to f$) according to the bounds of Sec. II.

3. Bounds for Zero Energy

In the limit $k \to 0$ one has $|j_l(x)| \to x^l/(2l+1)!!$ and $|h_l(x)| \to (2l-1)!!/x^{l+1}$. Using these expressions, we find

$$\alpha \leq \alpha^{(4)},$$

where

$$\alpha^{(4)}=(l+\tfrac{1}{2})^{-1}\beta_{1/2}, \quad k=0, \quad \text{and} \quad 0\leq\nu\leq l+1. \quad (4.22)$$

For $\nu \leq l$ this result was obtained by taking the zero-energy limit of Eq. (4.12); for $\nu=l+1$ one takes the limit of $\alpha^{(2)}$, Eq. (4.18).

The fact that $\alpha^{(4)}<1$ implies convergence is Kohn's result, (Ref. 11), his Eq. (11.2). For $\nu=l+1$, the zero-energy limit of our bound (2.15) is Kohn's Eq. (12.3).

4. Bounds Useful at Low Energies

In this case it is advantageous to put ν equal to $l+1$ or, if β_{l+1} does not exist, the highest value for which β_ν does exist. Again, all of the bounds of Sec. II are of interest. In particular, Eq. (2.17) becomes

$$|T_\infty| \leq 2[\pi(2l+1)!!(1-\alpha)]^{-1}\beta_{l+1}k^{2l+1}. \quad (4.23)$$

(If β_{l+1} does not exist, we get a corresponding result involving the factor $\beta_\nu k^{2\nu-1}$.)

This result should be compared with the familiar theorem[12] that, as $k \to 0$,

$$|T_\infty| \sim ck^{2l+1}, \quad (4.24)$$

where c is some constant. In making a comparison we note that this theorem is valid whenever β_{l+1} exists, whereas Eq. (4.23) has the shortcomings that it further requires $\alpha<1$ and does not rule out the possibility that $|T_\infty|$ will approach zero as k to some power higher than $(2l+1)$. On the other hand, our bound (4.23) is valid at all energies, while Eq. (4.24) is a statement only about the limit as $k \to 0$ (with the constant c undetermined); when one wants to apply this theorem for k small but nonzero, he has to somehow decide what constitutes being "close enough" to $k=0$.

5. Bounds Useful at High Energy

The appropriate choice in this case is $\nu=0$. Define the quantity, further discussed in Appendix 2,

$$A_l \equiv \max_{x,x'} xx'|j_l(x_<)h_l^{(1)}(x_>)|. \quad (4.25)$$

Equation (4.12) yields

$$\alpha \leq \alpha^{(5)},$$

with

$$\alpha^{(5)}=2A_l\beta_0 k^{-1} \quad (4.26)$$

(and $\nu=0$).

Note that $\alpha^{(5)} \to 0$ as $k \to \infty$ [as does $\|u_0\|$ of Eq. (4.15)]; we thus have the result that if β_0 exists, the Born expansion always converges for k sufficiently large[13]; in the limit $k \to \infty$ we further have $u_\infty \to u_1$ (and $u_1 \to 0$) according to the bounds of Sec. II. This statement is the analog of the result found for plane-wave scattering by Zemach and Klein.[9]

The above bound $\alpha \leq \alpha^{(5)}$ is valid for all energies. For the limit $k \to \infty$ one gets a somewhat sharper bound by using Eq. (4.18):

$$\alpha^{(2)} \to 2b_l(0)\beta_0 k^{-1}. \quad (4.27)$$

V. CONCLUDING REMARKS

In this paper we have restricted ourselves to the perturbation expansion for the scattering wave obeying boundary conditions stipulating an outgoing spherical wave, the asymptotic behavior of the wave function being given by the T matrix. Another perturbation expansion frequently encountered is that for a standing spherical wave[14] whose asymptotic behavior is given by the K matrix which, for partial waves, is the quantity

$$K_l=-\pi^{-1}\tan\delta. \quad (5.1)$$

We could equally well have applied the Banach-Weissinger theorem to obtain bounds for this case.

Instead of the iteration procedure (2.1),

$$F(\psi)=\psi_0+K\psi, \quad (5.2)$$

one can consider

$$G(\psi)\equiv F[F(\psi)]=\psi_0+K\psi_0+K^2\psi. \quad (5.3)$$

The sequence generated by $\psi_{n+1}=G(\psi_n)$ is a subsequence of that generated by $F(\psi)$; the Banach-Weissinger theorem applied to $G(\psi)$ yields bounds of higher precision than those obtained from $F(\psi)$. For plane-wave scattering this approach leads to a simplified derivation of the results of Zemach and Klein.[9]

A subject which should be investigated is the application of the Banach-Weissinger theorem to perturbation theory for bound states in quantum mechanics. In this case, one might take as a starting point the iteration procedure generating the perturbation expansion of Brillouin and Wigner[15]

$$F(\psi)=\psi_0+(1/E-H_0)\mathbf{P}V\psi, \quad (5.4)$$

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[12] See, for example, L. D. Landau and E. M. Lifshitz, *Quantum Mechanics* (Addison-Wesley Publishing Company, Inc., Reading, Massachusetts, 1958). The most general statement of this theorem seems to be by D. S. Carter, as quoted by R. G. Newton, J. Math. Phys. **1**, 319 (1960).

[13] The fact that β_0 finite implies that the Born expansion converges in the limit $k \to \infty$ is Kohn's result (Ref. 11), in his Eq. (11.8).

[14] Wu and Ohmura (Ref. 1), pp. 45 ff.; W. Kohn (Ref. 11), part I; L. Spruch (Ref. 8).

[15] P. M. Morse and H. Feshbach, *Methods of Theoretical Physics*, (McGraw-Hill Book Company, Inc., New York, 1953), Sec. 9.1 and the references cited there. Also see G. C. Wick, Rev. Mod. Phys. **27**, 339 (1955).

where $\mathbf{P}$ is the projection operator

$$\mathbf{P}=1-|\psi_0\rangle\langle\psi_0|. \quad (5.5)$$

APPENDIX I: THE BANACH-WEISSINGER THEOREM FOR ITERATIVE PROCESSES

The presentation here closely follows that of Collatz.[6] We recall the definition of a Banach space[16] $\mathcal{S}$ as being a normed linear space which is complete; that is, for every sequence $\{f_n\}$ in $\mathcal{S}$ with the property

$$\lim_{m,n\to\infty}\|f_m-f_n\|=0, \quad (A1.1)$$

there exists an element f, also in $\mathcal{S}$, with the property

$$\lim_{n\to\infty}\|f-f_n\|=0. \quad (A1.2)$$

Hilbert space is a particular case of a Banach space.

The Banach space of most interest to us here is the set of all functions $\psi(x)$ which are continuous over an arbitrary but fixed domain of the variable $x\equiv(x_1,x_2,\cdots,x_N)$; our norm will be

$$\|\psi\|=\max_x(|\psi(x)|/W(x)), \quad (A1.3)$$

where $W(x)$ is a fixed, positive, bounded, continuous, but otherwise arbitrary function. The following subspace is also a Banach space: the set of all continuous functions $\psi(x)$ lying within a sphere of radius R centered on some fixed element $\omega(x)$:

$$\|\psi-\omega\|\leq R. \quad (A1.4)$$

The demonstration that these are Banach spaces is elementary.[17] We also easily see that the wave functions of quantum mechanics constitute (or are embedded in) a Banach space.[18]

The Banach-Weissinger theorem can be stated as follows[3,6]: *Let F be a single-valued mapping of a Banach space $\mathcal{S}$ into itself which satisfies, for every f and g in $\mathcal{S}$, the Lipschitz condition*

$$\|F(f)-F(g)\|\leq\alpha\|f-g\| \quad (A1.5)$$

with

$$\alpha<1. \quad (A1.6)$$

Let f_0 be some element of $\mathcal{S}$, let f_1 be defined by $f_1=F(f_0)$, and suppose that $\|f_1-f_0\|$ is finite and that $\mathcal{S}$ contains all elements h in the sphere

$$\|h-f_1\|\leq\alpha(1-\alpha)^{-1}\|f_1-f_0\|. \quad (A1.7)$$

Then the sequence $f_0, f_1, f_2, \cdots$ defined by

$$f_{n+1}=F(f_n) \quad (A1.8)$$

is contained in the sphere (A1.7) *and converges [in the sense of* (A1.2)*] to a unique element f_∞ which lies in this sphere and has the property*

$$f_\infty=F(f_\infty). \quad (A1.9)$$

Furthermore,

$$\|f_\infty-f_n\|\leq\alpha(1-\alpha)^{-1}\|f_n-f_{n-1}\| \leq\alpha^n(1-\alpha)^{-1}\|f_1-f_0\|. \quad (A1.10)$$

Once the theorem is stated its proof is so simple we sketch it here: For $m>n$,

$$\|f_m-f_n\|\leq\|f_m-f_{m-1}\|+\|f_{m-1}-f_{m-2}\|+\cdots+\|f_{n+1}-f_n\| \leq(\alpha^{m-1}+\alpha^{m-2}+\cdots+\alpha^n)\|f_1-f_0\| \leq\alpha^n(1-\alpha)^{-1}\|f_1-f_0\|,$$

so the sequence $\{f_n\}$ satisfies (A1.1), thus implying the existence of a limit element f_∞ in $\mathcal{S}$. The above also shows that the entire sequence lies in the sphere (A1.7). It is then a simple exercise in epsilonics to show that the sphere also includes f_∞, that f_∞ satisfies (A1.9), and that f_∞ is unique. For $n=1$, Eq. (A1.10) then follows from Eq. (A1.7); this in turn implies Eq. (A1.10) for arbitrary n, as can be seen by thinking of starting the original iteration sequence with f_{n-1} instead of f_0.

APPENDIX 2: THE QUANTITIES $b_l(\nu)$, a_l, AND A_l

These quantities are defined by Eqs. (4.14), (4.20), and (4.25). $b_l(\frac{1}{2})$ is Kohn's m_l, while a_l^{-1} is his s_l.[19] Tables of these quantities can be constructed from tables of spherical Bessel functions; we give the results for the first few values of l in Tables I and II. In this

TABLE I. The quantity $b_l(\nu)=\max_x(j_l(x)/x^{\nu-1})$.

ν \ l	0	1	2	3
0	1.00000	1.06310	1.11082	1.14931
$\frac{1}{2}$	0.851241	0.658413	0.573257	0.520794
1	1.00000	0.436182	0.306792	0.241746
2		0.333333	0.104025	0.0574848
3			0.0666667	0.169359
4				0.00952381

TABLE II. The quantities $a_l=\max x|j_l(x)h_l^{(1)}(x)|$ and $A_l=\max x^2|j_l(x)h_l^{(1)}(x)|$.

\ l	0	1	2	3
a_l	1.00000	0.488633	0.359375	0.292746
A_l	1.00000	1.13302	1.24105	1.33218

[16] See, for example, I. N. Sneddon, *Handbuch der Physik*, edited by S. Flügge (Springer-Verlag, Berlin, 1955), Vol. II, p. 198.

[17] The key steps of this demonstration would involve using theorem (3.11) of W. Rudin, *Principles of Mathematical Analysis* (McGraw-Hill Book Company, Inc., New York, 1953), and constructing a proof similar to that of his theorem (7.12).

[18] Banach-space approaches to quantum mechanics have been used by W. Hunziker, Helv. Phys. Acta **34**, 593 (1961); J. G. Belinfante, J. Math. Phys. **5**, 1070 (1964); and C. Lovelace, Phys. Rev. **135**, B1225 (1964).

[19] W. Kohn (Ref. 11), Table V., Eq. (11.15), and Table VII.

connection, note that[10]

$$a_l = \max_x x |j_l(x) h_l^{(1)}(x)| \tag{A2.1}$$

and

$$A_l = \max_x x^2 |j_l(x) h_l^{(1)}(x)|\,. \tag{A2.2}$$

We also have

$$b_l(l+1) = 1/(2l+1)!!. \tag{A2.3}$$

For large l, one can use the asymptotic formula of Watson and Nicholson,[20] according to which

$$H_\lambda^{(1)}(x) \sim (3)^{-1/2} w H_{1/3}^{(1)}(y) \exp(i\tfrac{1}{6}\pi) \tag{A2.4}$$

as $l \to \infty$, where

$$\lambda \equiv l + \tfrac{1}{2},$$
$$y = \tfrac{1}{3}\lambda w^3,$$

and

$$w^2 = (x/\lambda)^2 - 1.$$

In writing this expression we used the fact that, for b_l, a_l, and A_l, the maximum is achieved for a value of y which tends to a constant as l tends to infinity; correspondingly, w tends to zero. We find that as $l \to \infty$

$$b_l(\nu) \sim 0.845843 (l+\tfrac{1}{2})^{1/6-\nu} (\nu < l+1)\,, \tag{A2.5}$$

$$a_l \sim 0.741397 (l+\tfrac{1}{2})^{-2/3}\,, \tag{A2.6}$$

and

$$A_l \sim 0.741397 (l+\tfrac{1}{2})^{1/3}\,. \tag{A2.7}$$

[20] W. Magnus and F. Oberhettinger, *Formulas and Theorems for the Functions of Mathematical Physics* (Chelsea Publishing Company, New York, 1954), Chap. 3, Sec. 3.

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Permutation Symmetry of Many-Particle Wave Functions*

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The symmetrization postulate (SP) states that wave functions are either completely symmetric or completely antisymmetric under permutations of identical particles. It is shown by one-dimensional counterexamples that SP is not demanded by the usual physical interpretation of the mathematical formalism of wave mechanics unless one makes use of further physical properties of real systems; the error in a standard proof of SP which ignores these properties is pointed out. It is then proved that SP is true for those systems of spinless particles which have the following properties: (a) probability densities are permutation-invariant, (b) allowable wave functions are continuous with continuous gradient, (c) the $3n$-dimensional configuration space is connected, (d) the Hamiltonian is symmetric, and (e) the nodes of allowed wave functions have certain properties. The counterexamples show that SP is not a necessary property of those systems which do not have property (c). The proof is extended to particles with internal degrees of freedom (including spin) by noting that any observable commutes with every permutation and making use of a particular observable acting only on internal variables. Extraneous mathematical assumptions, such as that of the existence of a "complete" set of commuting observables, criticized by Messiah and Greenberg, are not employed. Some comments are made on the conventional nature of the concept of identity for similar particles; the equivalence between the usual formulation in which different species of similar particles are treated as distinct, and that in which they are regarded as identical particles in different internal states, is emphasized.

1. INTRODUCTION

It is a well-known experimental fact that quantum-mechanical states of a system of identical elementary particles are either symmetrical (Bose-Einstein) or antisymmetrical (Fermi-Dirac) under permutations of the single-particle dynamical variables; more complicated permutation symmetries seem not to be realized in the real world. Messiah[1,2] calls this fact the *symmetrization postulate*. The pioneers in the development of quantum mechanics took this simply as an experimentally based fact. Thus, e.g., Dirac[3] states that: "Other more complicated kinds of symmetry are possible mathematically, but do not apply to any known particles." There were subsequent attempts, continuing up to the present time, to deduce the symmetrization postulate from other physical principles. One simple argument, found in many textbooks, runs as follows[4]: Let ψ be the Schrödinger wave function of a system of identical particles, let $P\psi$ be the wave function differing

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[1] A. Messiah, *Quantum Mechanics* (North-Holland Publishing Company, Amsterdam, 1962), Vol. II, p. 595.

[2] A. M. L. Messiah and O. Greenberg, Phys. Rev. **136**, B248 (1964).

[3] P. A. M. Dirac, *The Principles of Quantum Mechanics* (Clarendon Press, Oxford, 1947), 3rd ed., p. 211.

[4] See, e.g., E. M. Corson, *Perturbation Methods in the Quantum Mechanics of n-Electron Systems* (Blackie and Son, Ltd., Glasgow, 1951), p. 113.