The Scattering of Elementary Particles by Complex Nuclei—A Generalization of the Impulse Approximation

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By a systematic iteration procedure it is shown how the problem of the scattering of an elementary particle by a complex nucleus (or any many-particle target system) can be expressed in terms of two-body operators. The results are related to the previous work of Chew and Wick on the impulse approximation, with special attention given to multiple scattering effects which have heretofore not been formulated in a rigorous way. An explicit formula for the double scattering terms is presented.

I. INTRODUCTION

IN a recent paper,[1] hereafter referred to as I.A., Chew and Wick have presented a tentative analysis of the problem of the scattering of elementary particles by complex nuclei. They discuss the nature of the errors involved in treating such problems by the so-called "impulse approximation" introduced earlier by Chew.[2] The basic idea of this method may be stated as an attempt to represent the scattering amplitude from a complex nucleus as a superposition of scattering amplitudes from "free" nucleons which have the same momentum distribution as the initially bound nucleons. The assumptions under which the approximation is valid were stated to be the following: (I) The incident particle interacts only with one single nucleon at a time. (II) The amplitude of the incident wave is not appreciably diminished in crossing the nucleus. (III) The binding force has a negligible effect during the interval of strong interaction. Of these three assumptions, only (III) was discussed quantitatively in I.A. and even so, the mathematical treatment was based on a variational method which appeared unnecessarily devious. Shortly after the paper was submitted, Ashkin and Wick[3] succeeded in making a straightforward treatment of (III) for the case of the scattering by a single bound nucleon. The purpose of the present paper is to present a formal solution to the complete problem of expressing the scattering from a complex nucleus in terms of two particle operators. Our results include those of Ashkin and Wick as a special case and also permit a systematic discussion of assumptions (I) and (II).

II. FORMULATION AND SOLUTION OF THE PROBLEM

The problem is that of the scattering of a particle by a complex nucleus. The total Hamiltonian is (following the notation of I.A.)

$$H=H_0+V, \tag{1}$$

with

$$H_0=K+U. \tag{2}$$

K is the total kinetic energy operator, U the nuclear potential energy, and V is the total interaction between the nucleus and incoming particle. We shall suppose V to be of the form

$$V=\sum_{k=1}^{N} V_k, \tag{3}$$

where V_k is the interaction potential between the projectile and the kth nucleon. H_0 is the "unperturbed" Hamiltonian in terms of which the initial and final nucleus plus free particle states are classified. (We shall not be concerned here with the so-called pick-up processes in which the incident particle forms a bound state with one of the target nucleons). By adopting the formalism of Lippmann and Schwinger,[4] the exact solution of our problem may be expressed in terms of either of two state functions $\Psi_a^{(+)}$, $\Psi_b^{(-)}$ which satisfy the integral equations

$$\Psi_a^{(+)}=\Phi_a+\frac{1}{E_a+i\eta-H_0}V\Psi_a^{(+)}, \tag{4a}$$

$$\Psi_b^{(-)}=\Phi_b+\frac{1}{E_b-i\eta-H_0}V\Psi_b^{(-)}, \tag{4b}$$

where the Φ_a and Φ_b are eigenfunctions of H_0 belonging to the same energy E, the total energy of the system. In terms of these functions, the matrix elements of the operator T, the square of which is essentially the transition probability of interest, may be written as

$$T_{ba}=(\Phi_b, V\Psi_a^{(+)})=(\Psi_b^{(-)}, V\Phi_a), \tag{5}$$

with $E_a=E_b=E$.

We now replace the fundamental Eqs. (4) by operator

[1] G. F. Chew and G. C. Wick, Phys. Rev. **85**, 636 (1952).
[2] G. F. Chew, Phys. Rev. **80**, 196 (1950).
[3] J. Ashkin and G. C. Wick, Phys. Rev. **85**, 686 (1952).
[4] B. Lippmann and J. Schwinger, Phys. Rev. **79**, 481 (1950).

equations. Define two operators $\Omega^{(+)}$ and $\Omega^{(-)}$ by

$$\Omega^{(+)}\Phi_a=\Psi_a{}^{(+)}, \tag{6a}$$

$$\Omega^{(-)\dagger}\Phi_b=\Psi_b{}^{(-)}, \tag{6b}$$

where $\dagger$ means Hermitian adjoint. (We here deviate from the notation of I.A. where the symbol Ω is used to represent the operator designated in this paper by $\omega^{(+)}$.) The Φ are assumed to be a complete set so that (6) defines the operators $\Omega^{(\pm)}$. They satisfy the equations

$$\Omega^{(+)}=1+\frac{1}{E_a+i\eta-H_0}V\Omega^{(+)}, \tag{7a}$$

$$\Omega^{(-)}=1+\Omega^{(-)}V\frac{1}{E_b+i\eta-H_0}, \tag{7b}$$

so long as $\Omega^{(+)}$ is always going to operate on Φ_a to the right and $\Omega^{(-)}$ on $\Phi_b{}^*$ to the left. The operator Eqs. (7) may actually be freed of all reference to the states Φ_a and Φ_b by writing them as

$$\Omega^{(+)}=1-i\int_{-\infty}^{0}dxe^{\eta x}e^{iH_0x}V\Omega^{(+)}e^{-iH_0x}, \tag{8a}$$

$$\Omega^{(-)}=1-i\int_{-\infty}^{0}dxe^{\eta x}e^{-iH_0x}\Omega^{(-)}Ve^{iH_0x}. \tag{8b}$$

We shall continue, however, to use the forms given by (7) since there is no loss in generality.

In terms of $\Omega^{(\pm)}$ we may write expressions for operators $T^{(+)}$ and $T^{(-)}$ which have equal matrix elements between states Φ_a and Φ_b of the same energy and are both equal to the operator defined by Eq. (5) in such a case. We define

$$T^{(+)}=V\Omega^{(+)}, \tag{9a}$$

$$T^{(-)}=\Omega^{(-)}V. \tag{9b}$$

In the Appendix it is shown that, except for the time reversal unitary transformation, $\Omega^{(-)}$ is the transpose of $\Omega^{(+)}$ and $T^{(-)}$ is the transpose of $T^{(+)}$. Thus, it is really only necessary to write equations for the (+) operators. However, because the properties of the time reversal unitary transformation are familiar to only a small number of people, we have elected to write out the two equations in most cases.

The fundamental step of our development and the first original contribution of this paper is the recognition of the fact that the Eqs. (7) can be written in the form

$$\Omega^{(+)}=1+\frac{1}{E_a+i\eta-H_0-V}V, \tag{10a}$$

$$\Omega^{(-)}=1+V\frac{1}{E_b+i\eta-H_0-V}, \tag{10b}$$

as one may verify by expanding in powers of V and comparing with the iteration solution of Eqs. (7), or by operating on (10a), say with $(E_a+i\eta-H_0)^{-1}V$ and observing that the equation which results after some manipulation is just the first of Eqs. (7). It is clear that (10a) and (10b) may also be written

$$\Omega^{(+)}=1-i\int_{-\infty}^{0}dxe^{\eta x}e^{i(H_0+V)x}Ve^{-iH_0x}, \tag{11a}$$

$$\Omega^{(-)}=1-i\int_{-\infty}^{0}dxe^{\eta x}e^{-iH_0x}Ve^{i(H_0+V)x}. \tag{11b}$$

The physical meaning of the operators $\Omega^{(+)}$ and $\Omega^{(-)}$ is most clearly seen in the formalism of Ashkin and Wick,[3] who do not eliminate the time as we have done here. They show, for example, that if the system is in the state Φ_a "before" the collision, $\Omega^{(+)}$ is the operator which transforms Φ_a into the state $\Psi_b{}^{(+)}$ which exists "during" the collision. It is perhaps unfortunate that in the formalism used here, which deals with a stationary state of the system, the concept of collision time is obscure. The advantage of the stationary state approach, of course, is that one avoids the introduction of wave packets.

The forms of Eqs. (10) and (11) are such that we may easily develop an expansion of $\Omega^{(\pm)}$ (or $T^{(\pm)}$, using Eq. (9)) in powers of U. Such an expansion for the single scatterer problem was the object in I.A. and in the work of Wick and Ashkin.[3] The procedure of keeping only the zeroth-order terms of these expansions (terms independent of U) is quite properly referred to as the impulse approximation, since it corresponds to neglecting the effect of the binding field during the collision. However, when more than one target scatterer is present, as is always the case in a complex nucleus, the evaluation of these zeroth-order terms still requires solution of a many-body problem. We need to make a further approximation in order to obtain a workable formula, and the systematic formulation of this further approximation will be the second essential contribution of this paper.

The formal expression for the operator $T^{(+)}$ is

$$T^{(+)}=V+V\frac{1}{E_a+i\eta-H_0-V}V. \tag{12}$$

This expression, while exact and representing the formal solution of the complete problem, is of course not easily evaluable. We proceed then to rewrite (12) in a form suitable under certain conditions to an approximate evaluation. First we introduce the two particle scattering matrices $t_k{}^{(+)}$ and $t_k{}^{(-)}$ for the kth nucleon, defined by

$$(t_k{}^{(+)})_{mn}=(\chi_m, V_k\psi_{n,k}{}^{(+)}), \tag{13a}$$

$$(t_k{}^{(-)})_{mn}=(\psi_{m,k}{}^{(-)}, V_k\chi_n), \tag{13b}$$

where the ψ's are solutions of the equations

$$\psi_{l,k}{}^{(\pm)}=\chi_l+\frac{1}{E_l\pm i\eta-K}V_k\psi_{l,k}{}^{(\pm)}. \tag{14}$$

The χ's are eigenfunctions of K, and E_l is the eigenvalue of K belonging to χ_l. It is essential to differentiate between $t_k^{(+)}$ and $t_k^{(-)}$ since we require their matrix elements between states of unequal energy. We also introduce the analogs of Eqs. (9) and (10):

$$t_k^{(+)}=V_k\omega_k^{(+)}, \tag{15a}$$

$$t_k^{(-)}=\omega_k^{(-)}V_k, \tag{15b}$$

where

$$\omega_k^{(+)}=1+\frac{1}{E_l+i\eta-K-V_k}V_k, \tag{16a}$$

$$\omega_k^{(-)}=1+V_k\frac{1}{E_l+i\eta-K-V_k}. \tag{16b}$$

The validity of (16) requires $\omega_k^{(+)}$ to be operating to the right on χ_l and $\omega_k^{(-)}$ to be operating to the left on χ_l^*.

At this point a fundamental identity is to be derived. Let the symbol $B^{(+)}$ represent any operator of the form

$$B^{(+)}=\frac{1}{E_a+i\eta-H_0-V}A, \tag{17}$$

where A is an arbitrary operator. Let $b_k^{(+)}$ represent a corresponding operator,

$$b_k^{(+)}=\frac{1}{E_l+i\eta-K-V_k}A. \tag{18}$$

The relation between (17) and (18) is as follows:

$$B^{(+)}=b_k^{(+)}+(1/E_a+i\eta-H_0-V)\times\{[U,b_k^{(+)}]+(V-V_k)b_k^{(+)}\}. \tag{19a}$$

This identity is proved by the technique introduced in I.A., Eqs. (25) to (28). The method consists of writing $\Phi_a=\sum_l\chi_l(\chi_l,\Phi_a)$ and using the operator relation $(P-Q)^{-1}-P^{-1}=(P-Q)^{-1}QP^{-1}$, together with $H_0\Phi_a=E_a\Phi_a$. There also exists, of course, a relation corresponding to (19a) for $(-)$ type operators, $B^{(-)}=A(E_b+i\eta-H_0-V)^{-1}$:

$$B^{(-)}=b_k^{(-)}+\{[b_k^{(-)},U]+b_k^{(-)}(V-V_k)\}1/(E_b+i\eta-H_0-V). \tag{19b}$$

It is important to notice that the identities (19a) and (19b) can be used over and over again in a kind of iteration procedure.

To make a first application of our identities, let us rewrite Eq. (12) as

$$T^{(+)}=\sum_{k=1}^{N}\left\{V_k+V\frac{1}{E_a+i\eta-H_0-V}V_k\right\}. \tag{20}$$

We can apply (19a) to obtain

$$\frac{1}{E_a+i\eta-H_0-V}V_k=(\omega_k^{(+)}-1)+\frac{1}{E_a+i\eta-H_0-V}\times\{[U,\omega_k^{(+)}]+(V-V_k)(\omega_k^{(+)}-1)\},$$

which when substituted into (20) with a slight rearrangement of terms, yields

$$T^{(+)}=\sum_{k=1}^{N}\left\{t_k^{(+)}+V\frac{1}{E_a+i\eta-H_0-V}[U,\omega_k^{(+)}]+\left[1+V\frac{1}{E_a+i\eta-H_0-V}\right](V-V_k)(\omega_k^{(+)}-1)\right\}. \tag{21}$$

The importance of breaking up $T^{(+)}$ in this way is that often the part, $\sum_k t_k^{(+)}$, is much larger than the remaining two parts, and the operator, $t_k^{(+)}$, is relatively tractable, depending only on the kth target particle and the incident particle. An adequate and workable approximation in many cases is thus obtained by evaluating $\sum_k t_k^{(+)}$ exactly and either neglecting completely the last two parts of (21) or approximating them by further iteration as shown below.

The significance of the last two terms is suggested by the observation that in general when U vanishes, the term containing $[U,\omega_k^{(+)}]$ vanishes, while the other remains. On the other hand, when there is only a single target particle, the term containing $(V-V_k)(\omega_k^{(+)}-1)$ vanishes, independently of U. The connection with the arguments given in I.A. is, therefore, as follows: The term proportional to $[U,\omega_k^{(+)}]$ represents the error associated with assumption III, the impulse assumption. The term proportional to $(V-V_k)(\omega_k^{(+)}-1)$ combines the error due to assumptions I and II. We might call this either the multiple scattering error or the opacity error, neither name being perfect. One thing is clear at this point. The name "impulse approximation," which has been given to the procedure of neglecting *both* the last two parts of (21), is misleading, since it suggests that multiple scattering effects are not omitted.

III. THE ERROR CAUSED BY THE IMPULSE ASSUMPTION

By making use of (10b), (7b), and (9b) one sees that, for transitions to states Φ_b of the same energy as $\Phi_a(E_b=E_a=E)$, the second part of (21) is the same as the expression derived in I.A. for a single target particle:

$$V\frac{1}{E+i\eta-H_0-V}[U,\omega_k^{(+)}]=[\Omega^{(-)}-1][U,\omega_k^{(+)}]=T^{(-)}\frac{1}{E+i\eta-H_0}[U,\omega_k^{(+)}]. \tag{22}$$

A first approximation to (22) is obtained by application of (19b):

$$V\frac{1}{E+i\eta-H_0-V}=\sum_k V_k\frac{1}{E+i\eta-H_0-V}=\sum_k(\omega_k^{(-)}-1)+\sum_k\{[\omega_k^{(-)},U]+(\omega_k^{(-)}-1)(V-V_k)\}\frac{1}{E+i\eta-H_0-V}. \tag{23}$$

Regarding this as the second step of an iteration procedure, it is consistent to keep only the term $\sum_k(\omega_k^{(-)}-1)$ if the iteration is converging rapidly. Thus (22) is approximated by

$$\sum_k\sum_{k'}(\omega_{k'}^{(-)}-1)[U,\omega_k^{(+)}]$$
$$=\sum_k\sum_{k'}t_{k'}^{(-)}\frac{1}{E_l+i\eta-K}[U,\omega_k^{(+)}]. \quad (24)$$

The statements made in I.A. as to the conditions under which this error is small need no modification here. It should be noted that the result of Wick and Ashkin[3] corresponds to the original form of this term given in (21), i.e., the form which is valid for all matrix elements of $T^{(+)}$ and which may be expressed without reference to Φ_a as

$$-iV\int_{-\infty}^{0}dxe^{\eta x}e^{i(H_0+V)x}[U,\omega_k^{(+)}]e^{-iH_0x}. \quad (25)$$

IV. THE MULTIPLE SCATTERING ERROR

The third term of (21) can also be written in a variety of ways for transitions which conserve the energy, since

$$1+V\frac{1}{E+i\eta-H_0-V}=\Omega^{(-)}=T^{(-)}V^{-1}. \quad (26)$$

Thus, a possible form for the multiple scattering term in (21) is

$$\sum_{k=1}^{N}T^{(-)}V^{-1}(V-V_k)(\omega_k^{(+)}-1).$$

The following qualitative interpretation may be given this expression: The factor $(\omega_k^{(+)}-1)$ represents the outgoing wave from the kth nucleon. If the interaction between the incident particle and the individual nucleons is of short range in configuration space, then the dimensionless operator $V^{-1}(V-V_k)$ is localized at the positions of all the nucleons except the kth. Thus, the contribution of the kth term to the sum is proportional to the amplitude of the outgoing wave from the kth nucleon, evaluated at the positions of all the other nucleons. This is precisely the situation surmised on an intuitive basis in I.A. We have no reason to change the rough qualitative estimates made in that paper of the multiple scattering, but we can now give a formula suitable to quantitative calculation in the general case.

To obtain this formula, we carry out for the multiple scattering part of (21) the rearrangement (23) and again keep only the term $\sum_k(\omega_k^{(-)}-1)$. Thus, the multiple scattering term in first approximation is

$$[1+\sum_{k'}(\omega_{k'}^{(-)}-1)]\sum_k(V-V_k)(\omega_k^{(+)}-1). \quad (27)$$

Noticing that $\sum_k(V-V_k)(\omega_k^{(+)}-1)$ may be written $\sum\sum_{k\neq k''}V_{k''}(\omega_k^{(+)}-1)$, and remembering (15b), it is possible to re-express (27) as

$$\sum_{k'}\sum_{\neq k}t_{k'}^{(-)}(\omega_k^{(+)}-1)$$
$$+\sum_{k''}\sum_{\neq k'}\sum_{\neq k}(\omega_{k'}^{(-)}-1)V_{k''}(\omega_k^{(+)}-1). \quad (28)$$

The first part of (28) clearly represents double scattering, and this is, of course, very plausible as a next approximation to the single scattering terms $\sum_k t_k^{(+)}$. The second part of (28) involves three particles and should be neglected unless higher order terms are also kept in (23). Thus the final result for the first-order multiple scattering (double scattering) is

$$\sum_{k'}\sum_{\neq k}t_{k'}^{(-)}(\omega_k^{(+)}-1)$$
$$=\sum_{k'}\sum_{\neq k}t_{k'}^{(-)}\frac{1}{E_l+i\eta-K}t_k^{(+)}. \quad (29a)$$

It is worth recalling here a fact pointed out in I.A. We might just as well have begun by rearranging $T^{(-)}$ as $T^{(+)}$ and would then have arrived at $\sum_k t_k^{(-)}$ as a first approximation, with the double scattering term

$$\sum_{k'}\sum_{\neq k}(\omega_k^{(-)}-1)t_{k'}^{(+)} \quad (29b)$$

and the impulse correction term

$$\sum_k\sum_{k'}[\omega_k^{(-)},U](\omega_{k'}^{(+)}-1). \quad (30)$$

The two alternate forms are essentially the transposes of each other, and Blatt[5] has pointed out that if one wishes explicitly to maintain the property of detailed reversibility one should take the mean of the two. Actually, as shown by Ashkin and Wick,[3] the difference between the two is less than the residual error in the approximation.

APPENDIX

The material to be presented in this Appendix[6] is not intended to be an exhaustive discussion of the subject of time reversal but rather only to clarify the remarks made above. We assume that the Hamiltonian of our system may be written as $H=H_0+V$. If a system described by a state vector $\Psi(t)$ which satisfies the time dependent Schoedinger equation,

$$i\partial\Psi(t)/\partial t=H\Psi(t), \quad (A1)$$

is to be invariant under time reversal, then the state vector $\Psi(-t)$, which evidently satisfies

$$-i\partial\Psi(-t)/\partial t=H\Psi(-t), \quad (A2)$$

must be a possible solution of Eq. (A1). The appearance of the minus sign in (A2) suggests looking for the connection in the complex conjugate of (A1) [the state vectors $\Psi^*(t)$ must be regarded as being on an equal footing with the $\Psi(t)$], namely,

$$-i\partial\Psi^*(t)/\partial t=H^*\Psi^*(t). \quad (A3)$$

If then

$$\Psi(-t)=R\Psi^*(t), \quad (A4)$$

[5] J. M. Blatt, private communication.

[6] The notation employed here is largely based on unpublished notes of lectures given by J. Schwinger at Harvard in 1948.

where R is a unitary time independent operator which has the property

$$R^{-1}HR=R\dagger HR=H^*, \tag{A5}$$

Eq. (A2) becomes equivalent to (A3) and thus to (A1). We see then that the condition for invariance under time reversal is the existence of the operator R.

We now apply the results just derived to our problem. Specifically, we introduce "time reversed" states according to the definition

$$\Phi_{-b}\equiv R\Phi_b^*, \tag{A6}$$

where Φ_{-b} is the time reversed state corresponding to Φ_b. [For the simple case of a particle without spin, R is unity and if $\Phi_b=\exp(i\mathbf{k}\cdot\mathbf{r})$, $\Phi_{-b}=\exp(-i\mathbf{k}\cdot\mathbf{r})$ which evidently corresponds to a wave traveling in the opposite direction and hence with reversed velocity.] From our explicit equation for $\Omega^{(+)}$, namely,

$$\Omega^{(+)}=1+\frac{1}{E+i\eta-H}V, \tag{A7}$$

one finds using (A5)

$$R\dagger\Omega^{(+)}R=1+\frac{1}{E+i\eta-H^*}V^*=\Omega^{(-)T}, \tag{A8}$$

where we have assumed H_0 and V are hermitian and used the result

$$\Omega^{(-)}=1+V\frac{1}{E+i\eta-H}. \tag{A9}$$

This proves the remark made in the text following Eq. (9). Written more explicitly, Eq. (A8) furnishes the information

$$(\Phi_b, \Omega^{(-)}\Phi_a)=(\Phi_{-a}, \Omega^{(+)}\Phi_{-b}). \tag{A10}$$

As a further illustration of the interconnection between the various operators $T^{(\pm)}$ and state vectors $\Psi^{(\pm)}$ we note the following results:

$$\begin{aligned}\Psi_{-a}{}^{(+)}&=R\Psi_a{}^{(+)*}=\Omega^{(-)}\dagger\Phi_{-a},\\ \Psi_{-b}{}^{(-)}&=R\Psi_b{}^{(-)*}=\Omega^{(+)}\Phi_{-b}.\end{aligned} \tag{A11}$$

These express the not unexpected interchange of incoming and outgoing scattered waves. With (A11) it is easy to show that the usual form of the reciprocity law[4]

$$(\Psi_b{}^{(-)}, V\Phi_a)=(\Phi_b, V\Psi_a{}^{(+)}) \tag{A12}$$

takes on the form

$$(\Phi_{-a}, V\Omega^{(+)}\Phi_{-b})=(\Phi_b, V\Omega^{(+)}\Phi_a) \tag{A13}$$

or, in terms of $T^{(+)}=V\Omega^{(+)}$,

$$T_{-a,-b}{}^{(+)}=T_{b,a}{}^{(+)}. \tag{A14}$$

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An Application of the Cellular Method to Silicon*

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The calculations of Kimball and Mullaney applying the cellular method to elemental silicon are extended to a higher approximation. Although the energy gap is decreased through use of a larger number of harmonics, the values obtained are still much higher than that given by experiment. The proposal of Pearson, Haynes, and Shockley that the highest point of the filled band and the lowest point of the conduction band do not occur at the center of the zone may have a bearing on the results, since the calculations reported here are performed for zero wave number. The effective mass of the conduction electrons is determined under the assumption that the lowest point lies at the center of the zone.

INTRODUCTION

THE pure silicon crystal has the diamond type lattice and an experimentally known excitation energy as a semiconductor of 1.12 ev.[1] Kimball[2] obtained a solution for the band structure of diamond by use of the cellular method and Mullaney[3] adapted the diamond solution to silicon. Essentially the same method is used in part I of this paper to determine the lowest energy limit of the conduction band and the highest limit of the filled band, each for several possible values of the lattice spacing (under the assumption that the band limits occur at the center of the brillouin zone in a reduced scheme). The principal difference from previous work is in the choice of boundary conditions to be used in the fitting. In part II the functions obtained in part I are used to determine the effective mass for the conduction electrons.

The work reported here was performed in 1949 when it seemed likely that the top of the filled band and the bottom of the empty band did occur at the center of the brillouin zone. Pearson, Haynes, and Shockley have presented evidence[4] that these points may actually lie elsewhere in the brillouin zone. In spite of this, the calculations seem worth presenting briefly for their general value in connection with the properties of silicon.

I. THE BAND LIMITS

The total one electron eigenfunction may be expressed as[5]

$$\psi=\sum_l A_l[\sum_m C_{lm}Y_l{}^m(\phi,\theta)]R_l(E,r), \tag{1}$$

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