Approximate Reduction of the Many-Body Problem for Strongly Interacting Particles to a Problem of Self-Consistent Fields

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It is shown for systems of strongly interacting particles that in the limit of very many particles a transformation exists leading to an alternative problem which can be solved by a self-consistent field method. The transformed wave function describes "particles" moving in a collectively determined uniform potential; the transformation relating the transformed and original wave functions determines the amount of incoherence and correlation in the original function. The method appears to be more useful for fermion systems and is illustrated by applications to some aspects of nuclear structure.

I. INTRODUCTION

A WELL known approximation method for dealing with particles with weak or long-range interactions is the self-consistent field method of Hartree[1] and the related methods of Slater[2] and Fock.[3] It has in the past, however, been difficult or impossible to apply this method to systems of particles which interact strongly through short-range potentials. The origin of the difficulty lies in the strong correlations which must exist in the wave functions of the many-particle system, and which are neglected in the Hartree method. The great power of this method in its region of validity, however, shows the advantage of being able to construct a transformation which will bring the problem for strongly interacting systems into a form where the Hartree method can be applied. We shall now show that such a transformation does exist if we consider systems of many particles. The methods we use are based on a generalization and re-interpretation of a transformation introduced in another context by Francis and Watson.[4]

Before proceeding to the explicit discussion of this problem, we mention some qualitative features of approximations to certain well-known physical phenomena which suggest that the transformation which we seek in fact may at least approximately exist. First, it is well known from the study of nuclear structure that it is possible to introduce a formal model which predicts correctly a variety of details of the nuclear structure. This "shell model"[5] is based on the assumption that in some sense the effect of the many nuclear particles on a specified one may be represented by a collectively determined uniform potential. In this case each particle moves in a medium, the properties of which are determined by the states of the remaining particles. Consequently, since the state of the particle considered must be simply related to the states of the others, a problem of self-consistency arises. This requirement is usually only qualitatively stated and not in fact satisfied in many formulations of the nuclear problem. Applications of the ideas of this paper have, however, been previously made in papers[6] by the authors and are extended more generally in the following paper.[7]

Another variety of problems to which some features of the Hartree method apply is provided by the well known applications of the "optical" model.[8] In these cases the effects of localized strong interactions are replaced by an equivalent uniform potential; in most problems the effects of this potential on the states of the scattering system are ignored although if properly taken into account a problem of self consistency would arise.

Finally, a well-known application of a transformation to an equivalent problem in which a uniform potential acts on the particles is that used for a periodic lattice.[9] In this case the modulating effect of the lattice structure on the wave function can be transformed away (by introducing a function which is a product of a modulating function and a plane wave) and its effect replaced by an equivalent potential. In this case, as in the optical model, the lattice structure is assumed to be given and the effects of interactions is in first approximation ignored. The inclusion of these effects, however, would again give rise to a self-consistency problem, the determination of the lattice structure in a field which is in turn affected by the lattice structure.

With these qualitative remarks as an introduction, we proceed to the development of the method. In Sec. II we shall develop the formal properties of the transformation; in Sec. III we examine in detail the conditions under which the transformation is exact; in Sec. IV we discuss the characteristics of the transformation

[1] D. R. Hartree, Proc. Cambridge Phil. Soc. 24, 111 (1928).
[2] J. C. Slater, Phys. Rev. 35, 210 (1930).
[3] V. Fock, Z. Physik 61, 126 (1930).
[4] N. C. Francis and K. M. Watson, Phys. Rev. 92, 291 (1953).
[5] M. G. Mayer, Phys. Rev. 74, 235 (1948); Haxel, Jensen, and Suess, Phys. Rev. 75, 1766 (1949).

[6] Brueckner, Levinson, and Mahmond, Phys. Rev. 95, 219 (1954); K. A. Brueckner, Phys. Rev. 96, 908 (1954). These papers will be referred to henceforth as NS I and NS II, respectively.
[7] K. A. Brueckner, following paper [Phys. Rev. 97, 1353 (1955)]. This paper will be referred to henceforth as NS III.
[8] M. Lax, Revs. Modern Phys. 23, 287 (1951); L. Foldy, Phys Rev. 67, 107 (1945).
[9] F. Bloch, Z. Physik 52, 555 (1928).

to the coherent problem; in Sec. V we show that the solution may be formulated as a self-consistent problem; in Sec. VI we show to what extent this problem has the characteristics of a variational problem; in Sec. VII we discuss the physical interpretation of the transformed wave function and its relation to the physical wave function; finally in Sec. VIII we summarize our results and make some concluding remarks.

II. FORMALISM

In this section we shall examine in detail the nature of a transformation introduced by Francis and Watson[4] in their discussions of the many-body problem. We follow their notation and in much of this section we shall simply expand and comment on their derivation. In Appendix A we shall also give this derivation in an alternative form using the methods of second quantization. The necessary notation used there is less compact than that which we will use here; the more explicit representation of the operators, however, may give additional insight into the method.

The problem which we wish to solve is that of finding the eigenfunctions of the Hamiltonian

$$H = H_0 + \sum_\alpha v_\alpha, \qquad (1)$$

where H_0 is the sum of the kinetic energy operators and v_α is the potential energy of interaction for the αth pair. The sum over α is over all pairs, i.e.,

$$\sum_\alpha v_\alpha = \sum_{i<j} \sum v_{ij} = \frac{1}{2} \sum_i \sum_j v_{ij}. \qquad (2)$$

We shall now show that we can replace the problem of solving for the eigenfunctions of H by an alternative simpler problem.

Following Watson, we introduce the functions t_α and V_C defined in the following way:

$$t_\alpha = v_\alpha + v_\alpha \frac{P}{E - H_0 - V_C} t_\alpha, \qquad (3)$$

and

$$V_C = \sum_\alpha t_{C\alpha}, \qquad (4)$$

where $t_{C\alpha}$ is that part of the operator t_α which is diagonal with respect to the eigenstates of the operator $H_C = V_C + H_0$, i.e., the states defined by the equation

$$H_C \psi_C = (H_0 + V_C)\psi_C = E\psi_C. \qquad (4')$$

In Eq. (3) for t_α, $P(E - H_0 - V_C)^{-1}$ means that we take the principal value definition of the singularity. This is equivalent to omitting matrix elements to the ground state. The operator t_α is closely related to the scattering operator giving the scattering from the potential v_α, the only difference being the appearance of V_C in the energy denominator and the definition of the singularity.[10] The diagonal part of t_α is thus related to the forward scattering from the potential v_α.

[10] B. Lippmann and J. Schwinger, Phys. Rev. 79, 669 (1950).

To exhibit V_C in somewhat more compact form, we can combine Eqs. (3) and (4) for t_α and V_C into one equation by using first the result which follows from Eq. (1):

$$t_\alpha = v_\alpha + v_\alpha \frac{P}{E - H_0 - V_C - v_\alpha} v_\alpha, \qquad (5)$$

and inserting this into the definining equation for V_C. The result is

$$V_C = \sum_\alpha v_{C\alpha} + \left(v_\alpha \frac{P}{E - H_0 - V_C - v_\alpha} v_\alpha \right)_C, \qquad (6)$$

with the subscript C meaning diagonal with respect to the states ψ_C. This alternative defining equation for V_C is a nonlinear integral equation; we shall return to its implications and to a self-consistent method for solving it later. At present we shall proceed to evaluate the properties of the transformation operator which leads us to the potential.

We introduce the functions[†]

$$F = 1 + \frac{1}{e} \sum_\alpha I_\alpha F_\alpha,$$

$$\qquad (7)$$

$$F_\alpha = 1 + \frac{1}{e} \sum_{\alpha \neq \beta} I_\beta F_\beta,$$

where

$$I_\alpha = t_\alpha - t_{C\alpha}. \qquad (8)$$

The functions F and F_α thus depend only on the non-diagonal matrix elements of t_α except through the appearance of V_C in the energy denominators $e \equiv E - H_0 - V_c$. We finally construct a function

$$\varphi = F\psi_C. \qquad (9)$$

We wish to see to what extent the function φ is an eigenfunction of the original Hamiltonian. In the following we use the powerful symbolic methods of the operator algebra developed by Lippmann and Schwinger,[10] Chew and Goldberger,[11] and particularly by Watson.[12]

To carry out the desired proof, we consider first the product

$$\sum_\alpha v_\alpha F. \qquad (10)$$

By using the defining equation for F, this can be written

$$\sum_\alpha v_\alpha \left(1 + \frac{1}{e} \sum_\beta I_\beta F_\beta \right) = \sum_\alpha v_\alpha + \sum_\alpha v_\alpha \frac{1}{e} I_\alpha F_\alpha$$

$$+ \sum_{\alpha \neq \beta} \sum v_\alpha \frac{1}{e} I_\beta F_\beta. \qquad (11)$$

† *Note added in proof.*—The specification of principal value for the singularity in e^{-1} will be omitted here and in the following but must be included in an explicit evaluation.

[11] G. F. Chew and M. L. Goldberger, Phys. Rev. 87, 778 (1952).

[12] K. M. Watson, Phys. Rev. 89, 575 (1953).

The second term may be broken into two parts, i.e., we replace I_α by $t_\alpha - t_{C\alpha}$ [Eq. (8)]. We also make use of the relation between t_α and v_α stated in Eq. (3). We then find

$$v_\alpha \frac{1}{e} I_\alpha = v_\alpha \frac{1}{e}(t_\alpha - t_{C\alpha}) = t_\alpha - v_\alpha - v_\alpha \frac{1}{e} t_{C\alpha}. \quad (12)$$

We also use the identity

$$\sum_\alpha v_\alpha = \sum_\alpha v_\alpha \left(F_\alpha - \sum_{\beta \neq \alpha} \frac{1}{e} I_\beta F_\beta \right)$$

$$= \sum_\alpha v_\alpha F_\alpha - \sum_{\alpha \neq \beta} v_\alpha \frac{1}{e} I_\beta F_\beta. \quad (13)$$

Thus we can write Eq. (11), using Eq. (12), as

$$\sum_\alpha v_\alpha + \sum_\alpha \left(t_\alpha - v_\alpha - v_\alpha \frac{1}{e} t_{C\alpha} \right) F_\alpha + \sum_{\alpha \neq \beta} v_\alpha \frac{1}{e} I_\beta F_\beta$$

$$= \sum_\alpha v_\alpha F. \quad (14)$$

The first, third, and last terms of this combine by Eq. (13) to give zero. We also transform the second term by making use of first Eq. (8),

$$\sum_\beta t_\beta F_\beta = \sum_\beta (I_\beta + t_{C\beta}) F_\beta$$

$$= \sum_\beta I_\beta F_\beta + \sum_\beta t_{C\beta} + \sum_\beta t_{C\beta} (F_\beta - 1), \quad (15)$$

and then Eq. (7) for F_β in the last term, to give

$$\sum_\beta t_\beta F_\beta = \sum_\beta I_\beta F_\beta + \sum_\beta t_{C\beta} + \sum_{\alpha \neq \beta} t_{C\beta} \frac{1}{e} I_\alpha F_\alpha. \quad (16)$$

Combining this result with Eqs. (9), (10), and (14), we then find

$$\sum_\alpha v_\alpha \varphi = \left[\sum_\beta I_\beta F_\beta + \sum_\beta t_{C\beta} + \sum_{\alpha \neq \beta} t_{C\beta} \frac{1}{e} I_\alpha F_\alpha \right.$$

$$\left. - \sum_\beta V_\beta \frac{1}{e} t_{C\beta} F_\beta \right] \psi_C. \quad (17)$$

The second and third terms here can be combined by using Eq. (7):

$$\sum_\beta t_{C\beta} + \sum_{\alpha \neq \beta} t_{C\beta} \frac{1}{e} I_\alpha F_\alpha$$

$$= \sum_\alpha \sum_\beta t_{C\beta} \left(1 + \frac{1}{e} I_\alpha F_\alpha \right) - \sum_\beta t_{C\beta} \frac{1}{e} I_\beta F_\beta$$

$$= \sum_\beta t_{C\beta} F - \sum_\beta t_{C\beta} \frac{1}{e} I_\beta F_\beta. \quad (18)$$

For the first term of Eq. (17) we use (inserting principal

value explicitly)

$$(E - H_0 - V_C) F \psi_C = e \left(1 + \frac{P}{e} \sum_\alpha I_\alpha F_\alpha \right) \psi_C$$

$$= eP \frac{1}{e} \sum_\alpha I_\alpha F_\alpha \psi_C,$$

which follows from Eqs. (4') and (7). Thus we obtain the final result:

$$\sum_\alpha v_\alpha F \psi_C = (E - H_0 - V_C) F \psi_C + \sum_\beta t_{C\beta} F \psi_C$$

$$+ \left[1 - (E - H_0 - V_C) P \frac{1}{e} \right] \sum_\beta I_\beta F_\beta \psi_C$$

$$- \sum_\beta \left(t_{C\beta} \frac{1}{e} I_\beta + v_\beta \frac{1}{e} t_{C\beta} \right) F_\beta \psi_C.$$

By using the defining equation for V_C [Eq. (4)], this can also be written

$$(E - H_0 - \sum_\alpha v_\alpha) F \psi_C = \sum_\beta \left(t_{C\beta} \frac{1}{e} I_\beta + v_\beta \frac{1}{e} t_{C\beta} \right) F_\beta \psi_C$$

$$+ \left[(E - H_0 - V_C) P \frac{1}{e} - 1 \right] \sum_\beta I_\beta F_\beta \psi_C. \quad (19)$$

This result is in no sense an approximation; it follows as an identity from the definitions of Eqs. (3), (4), (7), and (9).

The last term of Eq. (19) is zero everywhere except on the energy shell since $(E - H_0 - V_C)^{-1} P (E - H_0 - V_C)^{-1}$ is equal to one everywhere except at $E = H_0 + V_C$ where $P(E - H_0 - V_C)^{-1}$ is equal to zero.[‡] The first two terms on the right side of Eq. (20) will be discussed in detail in the next section and shown to vanish as $1/N$ compared with the energy of the system. The only remaining correction to the energy which prevents $F \psi_i$ from being everywhere an exact solution in the limit $N \to \infty$ is the diagonal matrix element

$$\Delta E = \{ \psi_i, [1 - (E - H_0 - V_C) P (E - H_0 - V_C)^{-1}]$$

$$\times \sum_\beta I_\beta F_\beta \psi_C \} = (\psi_C, \sum_\beta I_\beta F_\beta \psi_C),$$

which gives in first nonvanishing order (inserting pair indices explicitly)

$$\Delta E = \sum_{i \neq j \neq k} \left(\psi_C, I_{ij} \frac{1}{e} I_{jk} \frac{1}{e} I_{kC} \psi_C \right). \quad (20)$$

The shift in the energy for a fermion system in a highly degenerate state which results from this correction has been evaluated in NS I and shown to give a very small

[‡] The authors are indebted to R. J. Eden and N. C. Francis and to F. E. Low and J. Bardeen who independently pointed out an error in a previous treatment of these terms.

effect. Thus we shall take the provisional view that the net effect of these high order correlation terms is small and examine the interpretation of the transformation and wave function neglecting the effects of these corrections. This assumption corresponds to the treatment used in the nuclear problems considered in NS I, II, and III, and allows us to exhibit more easily the structure and physical content of the method.

III. "1/N" CORRECTION TERMS

Dropping the correlation terms, we rewrite Eq. (19) in the form

$$(E-H)F\psi_C=\sum_\beta\left(t_{C\beta}\frac{1}{e}I_\beta+v_\beta\frac{1}{e}t_{C\beta}\right)F_\beta\psi_C\equiv H_1F\psi_C. \quad (21)$$

We thus can consider H_1 as defined by Eq. (21) to be a perturbing term in the Hamiltonian and determine its first order effect on the energy by evaluating the diagonal matrix elements of the perturbing energy.

We first bring the correction terms to more symmetric form by using the equations relating t, v, t_C, and I. We have an expansion for v_α in terms of t_α which follows from Eq. (3):

$$v_\alpha=t_\alpha-t_\alpha\frac{1}{e}t_\alpha+t_\alpha\frac{1}{e}t_\alpha\frac{1}{e}t_\alpha-\cdots. \quad (22)$$

Upon using this result, the two terms on the right side of Eq. (21) become:

$$\sum_\alpha\left[t_{C\alpha}\frac{1}{e}I_\alpha+t_{C\alpha}\frac{1}{e}t_{C\alpha}+I_\alpha\frac{1}{e}t_{C\alpha}-t_\alpha\frac{1}{e}t_\alpha\frac{1}{e}t_{C\alpha}+\cdots\right], \quad (23)$$

where we keep at present only the leading terms in the expansion. To evaluate the energy perturbation we also expand the F function in a power series in the incoherent scattering operator I_α, i.e., we expand Eq. (7) for F and F_α to give

$$F=1+\frac{1}{e}\sum_\alpha I_\alpha+\frac{1}{e}\left[\sum_{\alpha\neq\beta}\sum I_\alpha\frac{1}{e}I_\beta+\cdots,\right.$$

$$F_\alpha=1+\frac{1}{e}\sum_{\alpha\neq\beta}I_\beta+\frac{1}{e}\sum_{\alpha\neq\beta\neq\gamma}\sum I_\beta\frac{1}{e}I_\gamma+\cdots. \quad (24)$$

Using these expansions, we find to third order:

$$\Delta E_3=(F\psi_C,H_1F\psi_C)$$

$$=\sum_\alpha\left(\psi_C,\left[t_{C\alpha}\frac{1}{e}I_\alpha+t_{C\alpha}\frac{1}{e}t_{C\alpha}+I_\alpha\frac{1}{e}t_{C\alpha}-t_\alpha\frac{1}{e}t_\alpha\frac{1}{e}t_{C\alpha}\right.\right.$$

$$+\sum_\beta I_\beta\frac{1}{e}\left(t_{C\alpha}\frac{1}{e}I_\alpha+t_{C\alpha}\frac{1}{e}t_{C\alpha}+I_\alpha\frac{1}{e}t_{C\alpha}\right)$$

$$\left.\left.+\sum_{\beta\neq\alpha}\left(t_{C\alpha}\frac{1}{e}I_\alpha+t_{C\alpha}\frac{1}{e}t_{C\alpha}+I_\alpha\frac{1}{e}t_{C\alpha}\right)\frac{1}{e}I_\beta\right]\psi_C\right). \quad (25)$$

In this result most of the terms give no contribution; terms in which the combination $e^{-1}t_{C\alpha}\psi_C$) or $(\psi_C,t_{C\alpha}e^{-1}$ appears vanish since $t_{C\alpha}$ is diagonal in energy and the principal value treatment of the singularity in $1/e$ is equivalent to omitting the energy conserving part of $1/e$. Further we get contributions from terms involving pairs of operators I_α only if these operators act twice in the same pair of particles, the remaining combinations having no diagonal matrix elements. Using these two results Eq. (25) for the energy shift reduces to:

$$\Delta E_3=\sum_\alpha\left(\psi_C,I_\alpha\frac{1}{e}t_{C\alpha}\frac{1}{e}I_\alpha\psi_C\right). \quad (26)$$

This term is easily interpreted; it is the result of a scattering of the pair of particles out of the ground state ψ_C, their propagation and coherent scattering, and the final rescattering of the pair to their original state.

We can immediately draw a conclusion about the dependence of this term on the total number of particles N. We note that the operators t_C and I_α each contain a factor of v^{-1} (v the total volume) from the normalization of the wave functions. Further, the sum over intermediate momentum states contains a factor of v, since $\sum_k\rightarrow[v/(2\pi)^3]\int d\mathbf{k}$. The sum over all pairs of particles gives a factor $N(N-1)/2$. The net result is that

$$\Delta E_3=\tfrac{1}{2}N(N-1)v^{-2}f, \quad (27)$$

where f is a function independent of N. Since the total volume itself depends on N as:

$$v=N\Delta, \quad (28)$$

where Δ is the volume per particle, the energy shift is (for $N\gg1$):

$$\Delta E_3=\tfrac{1}{2}\Delta^{-2}f, \quad (29)$$

and is consequently independent of N. This is to be compared with the total energy E of the system which is proportional to N. We therefore see that the correction term ΔE_3 is indeed of order $1/N$ compared with the total energy.

It is important to note that this result depends in detail on the separation of t_α into $t_{C\alpha}$ and I_α, since it is the absence of diagonal elements in I_α which suppresses the magnitude of the energy shift. For any other choice of I_α, the second order terms in the perturbing energy would not vanish and corrections of order N rather than of order unity would appear.

It is of interest to exhibit explicitly the magnitude of these "1/N" terms. We have done this in Appendix B in the case which is of particular interest to us, i.e., the nuclear structure problem. Using a simplified model we have found that the energy shift per particle resulting from the perturbing terms is approximately 10 Mev/N. This is quite negligible (for moderate values of N) compared with the unperturbed energy per particles of about -14 Mev.

It is easy to show by inspection of the next terms in the expansion of the perturbing energy that their matrix elements are also independent of N or depend on powers of $1/N$; they therefore also vanish compared with the unperturbed energy as $N \to \infty$. The only remaining question concerns the convergence of the expansion in $t_{C\alpha}$ and I_α which we have used. It is not easy to estimate the general term in this series which contains multiple combinations of incoherent and coherent scatterings. We have, however, examined the next term of fourth order, which can be shown to be:

$$\Delta E_4 = \left(\psi_C, \left\{ \sum_{\alpha \neq \beta \neq \gamma} \sum \sum \left[I_\alpha \frac{1}{e} t_{C\alpha} \frac{1}{e} I_\beta \frac{1}{e} I_\gamma + I_\alpha \frac{1}{e} t_{C\beta} \frac{1}{e} I_\beta \frac{1}{e} I_\gamma \right. \right. \right.$$
$$\left. + I_\alpha \frac{1}{e} I_\beta \frac{1}{e} t_{C\beta} \frac{1}{e} I_\gamma + I_\alpha \frac{1}{e} I_\beta \frac{1}{e} t_{C\gamma} \frac{1}{e} I_\gamma \right]$$
$$\left. \left. + \sum_\alpha \sum_\beta \left[I_\alpha \frac{1}{e} t_{C\beta} \frac{1}{e} t_{C\beta} \frac{1}{e} I_\alpha \right] \right\} \psi_C \right). \quad (30)$$

Part of the last term here arises from the second order perturbation of H_1 [see Eq. (21)]; it is easily shown using the arguments used to evaluate the N dependence of ΔE_3 to be of order $1/N$ and hence to be negligible. We consider the remaining terms in more detail. They are closely related to the energy perturbation evaluated in the nuclear case in NS I[6] except for the presence of a term $t_{C\alpha}/e$. This we approximate rather roughly as being of the order $1/N$. The remaining sum over α, β, γ is identical with the expression evaluated in NS I which was found to give very approximately 0.15 Mev per particle. Thus we have, in order of magnitude,

$$\Delta E_4 \approx (1/N)(0.15 \text{ Mev} \times N) = 0.15 \text{ Mev}. \quad (31)$$

This is much smaller than the lowest order perturbation, $\Delta E_3 \approx 10$ Mev; we therefore have some indication of a very rapid convergence of the expansion of Eq. (23) for the perturbing energy.

IV. INTERPRETATION OF THE TRANSFORMATION FUNCTION F

Restating the conclusion of the last section; we find (to the approximation discussed at the end of Sec. II) that

$$\varphi = F\psi_C \underset{N \to \infty}{=} \psi, \quad (32)$$

where ψ is an eigenfunction of H belonging to the energy E and ψ_C is an eigenfunction of H_C belonging to the same eigenvalue. We can easily derive an equivalent formal statement of this result. Let us introduce F^{-1}, the inverse of F. Then we have

$$E\psi_C = H_C\psi_C. \quad (33)$$

Multiplying by F, this becomes

$$FE\psi_C = EF\psi_C = FH_C\psi_C = FH_CF^{-1}F\psi_C. \quad (34)$$

Since $F\psi_C$ is the wave function ψ (in the limit as $N \to \infty$), this can be written as

$$E\psi = (FH_CF^{-1})\psi. \quad (35)$$

Thus we are led to identify FH_CF^{-1} with the Hamiltonian, i.e.,

$$FH_CF^{-1} = H \quad (36)$$

or

$$H_C = F^{-1}HF. \quad (37)$$

The function F therefore acts as a transformation on the wave function; the solution of the original problem for the eigenvalue is equivalent to the solution of the transformed problem with the transformed Hamiltonian H_C.

A difficulty not so far stated but implicit in these results arises from the specification of the boundary values in the transformed problem. We are interested in a bound system and it would perhaps seem sufficient to specify the vanishing of the wave functions on some boundary, thus approximating in the solution for H_C to the appearance of a surface in the actual solution for ψ. This cannot, however, be generally correct since the function F depends nonlocally on the coordinates of the particles and so can introduce a difference in the boundary conditions for ψ and ψ_C. It is thus important to show that the separation $t_\alpha = t_{C\alpha} + I_\alpha$ has been made in such a way as to minimize this boundary condition effect. That this is so is rather obvious in the nuclear problem in which we consider a highly degenerate Fermi gas. As a result of the action of the exclusion principle the incoherent operators I_α have matrix elements from the ground state only to excited states in which the excited particles occupy previously empty states. The associated large momentum transfers and large excitation energies can both be expected to reduce very considerably the effects of incoherence and thus to make F approximately an identity operator for states below the Fermi momentum.

Thus we see that in many ways the separation which we have made is an optimum one; not only is the transformed problem in H_C much more easily soluble than the original problem but also the effects of F in the fermion case are perhaps as small as the simpler choices of I_α will allow. We note that these remarks do not hold for a system of bosons where the exclusion principle cannot act to simplify the effects of F.

V. SELF-CONSISTENT APPROXIMATION METHOD

We restate the result of the preceding sections, which is that we can determine the energy eigenvalues by solution of the eigenvalue problem,

$$E\psi_C = (H_0 + V_C)\psi_C, \quad (38)$$

with V_C defined by Eqs. (3) and (4). Let us examine the definition more closely; first, we note that the

definition[13] of t_α,

$$t_\alpha = v_\alpha + v_\alpha (E - H_0 - V_C)^{-1} t_\alpha, \qquad (39)$$

involves V_C. Further, the definition of V_C involves evaluation of the diagonal matrix elements of t_α with respect to the unknown states ψ_C. Thus these definitions are obviously not fully specified, and a problem arises of choosing the states ψ_C and the potential V_C in such a way that the set of coupled equations for V_C and ψ_C are satisfied. A suitable self-consistent method is the following:

(1) Assume a set of states $\psi_C{}^{(0)}$ which are product functions of the variables of N particles, and a potential $V_C{}^{(0)}$ diagonal with respect to these states.

(2) Use Eq. (3) to calculate $t_\alpha{}^{(0)}$ and from this compute $t_{C\alpha}{}^{(0)}$ using the assumed definition of the states $\psi_C{}^{(0)}$.

(3) Construct $V_C{}^{(1)}$ from the computed $t_{C\alpha}{}^{(0)}$ and finally determine the eigenstates $\psi_C{}^{(1)}$.

(4) Compare the eigenstates $\psi_C{}^{(1)}$ with $\psi_C{}^{(0)}$ and the potential $V_C{}^{(1)}$ with $V_C{}^{(0)}$.

(5) Adjust the choices of states and V_C and recycle through steps 1–4.

This procedure is troubled by the same questions of convergency and stability that occur in the Hartree method. In the case of a semi-infinite medium, however, the procedure is greatly simplified since the states ψ_C are exactly known, namely, properly symmetrized product plane wave states. The potential V_C diagonal with respect to these states is simply diagonal in momentum space. An approximate solution to the self-consistency problem has been obtained for the nuclear structure case in NS III[7] and is discussed in detail there.

VI. VARIATIONAL ASPECTS OF THE PROBLEM

With the choice of the transformation function F which we have discussed in Secs. II, III, and IV, we see that ψ_C, describing as it does plane wave motion, can be written as a product of plane wave functions. The potential energy of the system can then be evaluated by carrying out the sum over the forward scattering amplitudes. This, however, is in some ways not closely related to the physical problem since the actual solution ψ for a bound system predicts a closed surface which cannot be given by the transformed Hamiltonian H_C. To approximate to the physical state, we thus are forced to specify boundary conditions for ψ_C which represent the effects of the surface. This can be done by requiring that the transformed wave function satisfy periodic boundary conditions or vanish on the surfaces of a normalization volume. For the nuclear case discussed in detail elsewhere, we have specified that the wave function vanish on the surface of a sphere.

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[13] See also Appendix A for the modification of this operator for the case of many fermions. The change discussed there is equivalent to the omission of certain intermediate states in the summation implied in Eq. (39).

Further, since the energy of the system is a minimum when the physical system takes on its stable density, we regard the density a parameter to be varied until the energy is a minimum. In this way we assume that we approximate closely to the physical situation; one can also describe this procedure as a variational problem of standard form in which the trial function is $\varphi = F\psi_C$ and the density ρ is a variational parameter.

Let us consider the variational aspects of the problem more fully: We let ψ_0 be the true eigenfunction of the system with eigenvalue E. Introducing our approximate $\varphi = F\psi_C$ with a variational parameter ρ (the density) contained in the specification of ψ_C, we have

$$E_0 \leq (\varphi, H\varphi)/(\varphi, \varphi) = E(\rho). \qquad (40)$$

Making use of the transformation properties of F, this can be written as

$$\begin{aligned}
E(\rho) &= \frac{(F\psi_C, HF\psi_C)}{(F\psi_C, F\psi_C)} = \frac{(\psi_C, F^\dagger HF\psi_C)}{(\psi_C, F^\dagger F\psi_C)} \\
&\underset{N\to\infty}{=} \frac{(\psi_C, F^\dagger FH_C\psi_C)}{(\psi_C, F^\dagger F\psi_C)} = E_C = \frac{(\psi_C, H_C\psi_C)}{(\psi_C, \psi_C)}, \qquad (41)
\end{aligned}$$

again neglecting the high order correlation terms and the correction terms which vanish for large N. The function F contains all the correlations in the system; the ψ_C is an uncorrelated product of plane wave functions. This is very similar to the form introduced by Bloch[9] and also to that used by Drell and Huang[14] in the nuclear problem; the particular form which we have chosen, however, allows us to make the transformation of Eq. (41) so that we are able to replace the problem of determining ψ by the simpler problem of determining ψ_C. We observe one very simple feature of these results, which is that we do not need an explicit form for F [other than the formal definition of Eq. (7)] to evaluate the energy $E_C(\rho)$, since we have an explicit form H_C for the transformed Hamiltonian $F^{-1}HF$.

VII. RELATION BETWEEN ψ_C AND ψ

It is important to remark that the relation between the actual wave function ψ and the "coherent" ψ_C is not simple since it involves the operator F which is known only formally through the defining equations [Eq. (7)]. We can, however, see several obvious features of ψ if we examine the lowest term in the incoherent scattering operators I_α in the expansion for F, which is

$$\psi = F\psi_C = \psi_C + \frac{1}{e} \sum_\alpha I_\alpha \psi_C + \cdots. \qquad (42)$$

The leading term shows that the actual wave function contains an admixture of single-particle states, the predominance of this state depending on the matrix ele-

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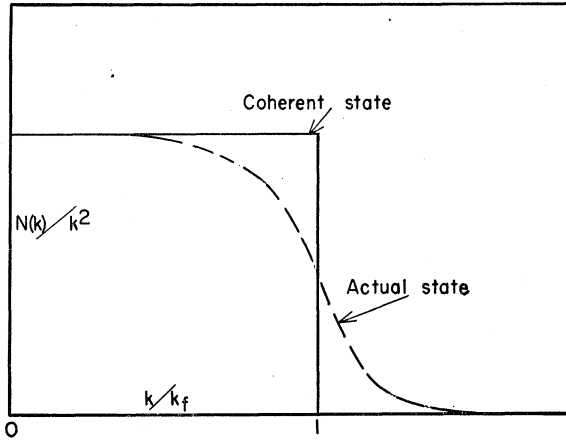[14] S. D. Drell and Kerson Huang, Phys. Rev. **91**, 1527 (1953).

FIG. 1. Departure of lowest energy state ψ for a highly degenerate fermion gas from the state ψ_C.

ments of I_α for excitations of the nucleus. The effect of the term in the incoherent scattering operator I_α is to mix into the wave function excited states in which two particles at a time have been excited; if we fix our attention on a state ψ in which a given pair have been excited, then we find contributions to this state by evaluating the matrix elements of I_α between the desired state and all unexcited states. In a fermion gas we expect the effect to be largest on states just below the Fermi momentum since the matrix elements of I_α are then the largest. The energy denominator also varies rapidly with particle excitation, particularly because of the modified mass effect[7] which very considerably increases the kinetic energies. This is equivalent to including the effect of the rapid decrease of the potential (see NS II and III) felt by a particle as it goes into excited states. The higher terms in the expansion of F also have an obvious interpretation; they are associated with further incoherent scatterings which could lead to additional excitations of the system or to repopulation of the low-lying empty states.

Typically we might expect for a degenerate Fermi gas an effect of the sort shown in Fig. 1, the actual state ψ approximating fairly well to the state ψ_C for momenta below the Fermi momentum, but showing an admixture of higher-momentum states. Although the effect of these on, for example, the mean energy of the system is in our formulation zero, we would expect that under certain circumstances the appearance of very high Fourier components in the wave function would strongly manifest itself. This would be, for example, in high-energy processes depending critically on the high-momentum components, where the almost fully populated low-lying momentum states would have little effect and consequently a small admixture of high-momentum states would have great importance.

These results are not at all unexpected in the case of nuclear structure, since it is well known that the shell model is only a first approximation to a correct de-

scription of the nucleus, the perturbing effects on the surface states of two-body interactions being rather important. We see that the independent-particle model may give a good representation of certain properties of the nucleus (such as the ordering of states and mean energy, for example) but be quite inadequate for other properties dealing with finer details of the structure.

VIII. SUMMARY OF RESULTS AND CONCLUSIONS

In this paper we have examined the nature of the method which was introduced by Watson and Francis[4] in the study of the optical model and which we have generalized to apply to strongly correlated many-particle systems. This method is in essence the replacement of the original problem by an alternative simpler problem which arises from the original one by the transformation discussed in the preceding sections. This transformation is, as we have seen, exact as the number of particles become very large if the correlation terms discussed earlier are neglected. The transformed "coherent" problem is relatively easy to solve except for an uncertainty in the proper boundary conditions; its solution has been discussed in NS I, NS II, and NS III. The treatment of the boundary is difficult in the transformed problem; we have discussed the replacement of the physical surface by a boundary condition on the wave functions which lead to a variational problem for the energy. The "independent particle" wave function ψ_C, which arises naturally in the transformed problem, cannot be directly interpreted as the physical wave function since the latter is obtained from the former by a transformation which introduces correlations into the wave function. As a consequence, in the case of a nucleus the system departs from a Fermi gas in that, for example, higher-momentum components are present in the wave function. Reasons are discussed, however, which show that in considerations of certain general features of the nucleus, the actual wave function may be identified with the independent-particle function ψ_C. We expect, however, that the departures of the structure from a true independent-particle structure cannot be neglected for high-energy phenomena.

A dominant feature of the method we have described is that it has at present been shown to give only the correct lowest energy eigenvalue with good accuracy, this being the result of our obtaining an explicit (and simple) representation for the transformed Hamiltonian H_C. It is possible, however, that other quantum numbers of the transformed problem (such as parity and angular momentum) may also be simply related to the quantum numbers of the physical system, i.e., that it may be able to exhibit simply the transformed angular momentum and parity operators. These and similar questions are to be discussed in detail, together with the properties of more general transformations than we have considered, by Eden and Francis.[15]

[15] R. J. Eden and N. C. Francis, this issue [Phys. Rev. 97, 1366 (1955)].

APPENDIX A

Diagonalization of the Hamiltonian in Second-Quantized Form

We introduce a set of basis states φ_i and write the Hamiltonian as a second-quantized operator on the occupation numbers of these states, i.e., we have (with T_i the kinetic energy in the ith state):

$$H = \sum_i T_i \eta_i^* \eta_i + \tfrac{1}{2} \sum_{ijkl} v_{ij,kl} \eta_i^* \eta_j^* \eta_l \eta_k = H_0 + V, \quad (A1)$$

where the η_i and η_i^* are annihilation and creation operators with commutation laws (for a system of fermions):

$$[\eta_i, \eta_j^*]_+ = \delta_{ij}. \quad (A2)$$

The change for boson systems is of course made by replacing the anticommutator by the commutator.

We seek a transformation which will transform H into an operator with only diagonal matrix elements. In analogy with Sec. II, we introduce the scattering operator:

$$t_{ij,kl} = v_{ij,kl} + \sum_{mn} v_{ij,mn} \eta_m \eta_n \frac{1}{e} \eta_n^* \eta_m^* t_{mn,kl}. \quad (A3)$$

We also as before break this into a diagonal and non-diagonal part:

$$t_{ij,kl} = t_{ij,ij} \delta_{ik} \delta_{jl} + t_{ij,ji} \delta_{kj} \delta_{il} + I_{ij,kl}, \quad (A4)$$

and use this to define the diagonal operator:

$$e = E - \sum_i T_i \eta_i^* \eta_i - V_C, \quad (A5)$$

where E is the energy eigenvalue and

$$V_C = \tfrac{1}{2} \sum_{ij} (t_{ij,ij} \eta_i \eta_j \eta_j^* \eta_i^* + t_{ij,ji} \eta_i \eta_j \eta_i^* \eta_j^*). \quad (A6)$$

Finally, using the definition of $I_{ij,kl}$ given in Eq. (A4), we construct the operators F and F_{kl} by using the equations:

$$F = 1 + \frac{1}{e} \sum_{ijkl} I_{ij,kl} \eta_i^* \eta_j^* \eta_l \eta_k F_{kl},$$

$$\quad (A7)$$

$$F_{kj} = 1 + \frac{1}{e} \sum_{ij \neq kl} \sum_{mn} I_{ij,mn} \eta_i^* \eta_j^* \eta_n \eta_m F_{mn}.$$

We next proceed to the proof of the desired result. The development follows rather closely the more general technique used in Sec. II and consequently we shall somewhat condense our arguments. First we consider the sum:

$$\tfrac{1}{2} \sum_{ijkl} v_{ij,kl} \eta_i^* \eta_j^* \eta_l \eta_k F = VF. \quad (A8)$$

By using the definitions of the various operators and proceeding in a way very similar to that used in Sec. II,

this can easily be brought to the form

$$VF = \tfrac{1}{2} \sum_{ijkl} t_{ij,kl} \eta_i^* \eta_j^* \eta_l \eta_k F_{kl}$$

$$- \tfrac{1}{2} \sum_{ijkl} v_{ij,kl} \eta_k^* \eta_l^* \frac{1}{e} (t_{kl,kl} \eta_l \eta_k + t_{kl,lk} \eta_k \eta_l) F_{kl}. \quad (A9)$$

The last term here is of the type that has been shown to vanish for large numbers and will be dropped. The remaining term breaks into two parts:

$$VF = \tfrac{1}{2} \sum_{ij} (t_{ij,ij} \eta_i^* \eta_j^* \eta_j \eta_i + t_{ij,ji} \eta_i^* \eta_j^* \eta_i \eta_j) F_{ij}$$

$$+ \tfrac{1}{2} \sum_{ijkl} I_{ij,kl} \eta_i^* \eta_j^* \eta_l \eta_k F_{kl}. \quad (A10)$$

To eliminate the second of these, we define a state function Ψ_0 such that $e = E - H_0 - V_C$ operating on it vanishes. Using this and the defining equation for F [Eq. (A7)], we finally find

$$VF\Psi_0 = (E - H_0) F\Psi_0, \quad (A11)$$

if we again drop a term which vanishes for a large number of particles. The state function $F\Psi_0$ thus satisfies the original eigenvalue equation for the energy if the auxiliary equation,

$$(H_0 + V_C)\Psi_0 = E\Psi_0, \quad (A12)$$

is satisfied. This equation for Ψ_0 replaces the original eigenvalue problem for E. The evaluation of the eigenvalue is now relatively easy if we know the operators $t_{ij,kl}$, since for the lowest eigenvalue of E we choose a Ψ_0 in which the states are all occupied, i.e., a degenerate gas.

Returning to the equation for $t_{ij,kl}$, a typical diagonal term is

$$t_{ij,ij} = v_{ij,ij} + v_{ij,mn} \eta_m \eta_n \frac{1}{e} \eta_n^* \eta_m^* t_{mn,ij}. \quad (A13)$$

When we operate on the initial state Ψ_0, the second term vanishes unless the particles m and n which are created occupy previously empty states. In this case, the matrix element of $\eta_m \eta_n \eta_n^* \eta_m^*$ is simply unity. The energy denominator then contains the difference between the energy E of the initial state and the energy of the excited state with the two particles m and n excited. Writing the energies in terms of H_0 and V_C, this difference may be written

$$\Delta E = T_i + T_j - T_m - T_n + V_C(i)$$
$$+ V_C(j) - V_C(m) - V_C(n), \quad (A14)$$

where

$$V_C(i) = \sum_{s \neq i} (t_{is,is} - t_{is,si}), \quad (A15)$$

again dropping terms which vanish for large numbers. Thus the energy denominator depends explicitly only on the coordinates of the initial and excited pairs of particles, although it depends implicitly on the states of the rest of the particles through the sum over the filled states of the rest of the system.

We also note the iterated form of F:

$$F = 1 + \frac{1}{e} \sum_{ij,kl} I_{ij,kl} \eta_i^* \eta_j^* \eta_l \eta_k$$

$$+ \frac{1}{e} \sum_{ij,kl} I_{ij,kl} \frac{1}{e} \eta_i^* \eta_j^* \eta_l \eta_k \sum_{mn \neq kl} \sum_{rs} I_{mn,rs}$$

$$\times \eta_m^* \eta_n^* \eta_s \eta_r + \cdots. \quad (A16)$$

This has no diagonal elements in the state Ψ_0 until the fourth term of order I^3 is taken into account. This result has been already used in NS I.

We also consider in this notation a typical $1/N$ term discussed in Sec. III and also in Appendix B:

$$\left(\psi_C, \sum_{\alpha\beta} I_\alpha \frac{1}{e} t_{C\alpha} \frac{1}{e} I_\beta \psi_C \right).$$

In the second quantization notation, this is

$$\sum_{ijkl} \sum_{k'l'mn} (\Psi_0, \eta_i^* \eta_j^* \eta_l \eta_k \eta_k^* \eta_i^* \eta_l \eta_k \eta_{k'}^* \eta_{l'}^* \eta_n \eta_m \Psi_0)$$

$$\times I_{ij,kl} \frac{1}{e} (t_{kl,kl} - t_{kl,lk}) \frac{1}{e} I_{k'l',mn}.$$

In evaluating the matrix element of the annihilation and creation operators, the restriction on the sum over operators associated with the nondiagonal operators I shows that the only diagonal terms can come from pairing the annihilation and creation operators $(\eta_l \eta_k \eta_{k'}^* \eta_{l'}^*)$ to give a diagonal contribution, i.e., the particles created by $\eta_{k'}^* \eta_{l'}^*$ must be annihilated by the pair $\eta_l \eta_k$. Thus the summation over k' and l' is restricted to the diagonal terms; a similar restriction occurs in the summation over i, j, m, n. A typical resulting term is

$$\sum_{ijkl} \left(I_{ij,kl} \frac{1}{e} t_{kl,kl} \frac{1}{e} I_{kl,ij} \right)$$

together with a variety of exchange terms. This term has the structure of the terms discussed in Sec. III and evaluated in Appendix B; thus the arguments showing the vanishing of these terms for large N go through as before.

APPENDIX B

Approximate Evaluation of ΔE_3

We wish to evaluate the first nonvanishing perturbation in the energy:

$$\Delta E_3 = \sum_\alpha \left(\psi_C, I_\alpha \frac{1}{e} t_{C\alpha} \frac{1}{e} I_\alpha \psi_C \right). \quad (B1)$$

We consider as an explicit case the nuclear system. As discussed in Sec. III this term represents the incoherent scattering of a pair of particles to excited states, their coherent scattering, and final rescattering to the

original state. We shall try to obtain only a qualitative result since, as we have shown, the effect on the energy is very small. Consequently we shall replace the exact expression by a simpler one in which we treat the pair as a single particle with mass equal to the reduced mass of the pair. We also consider the relative momentum as the momentum of a physical particle and require that it be above the Fermi momentum in the excited states. With these approximations we can write for a typical "particle" (i.e., pair):

$$\Delta E_3 = \sum_{k', |k'| > k_F} (k | I | k') \frac{M^*}{k^2 - k'^2} (k' | t_C | k')$$

$$\times \frac{M^*}{k^2 - k'^2} (k' | I | k), \quad (B2)$$

where we have approximated the effect of V_C in the denominator $1/e$ by a mass modification as discussed in NS III. For simplicity we choose for $(k'|t|k)$ the Born approximation scattering from a Yukawa well with Serber exchange mixture, i.e., we let

$$V(r) = V_0 \frac{e^{-\mu r}}{\mu r} \frac{1}{2}(1 + P_x), \quad (B3)$$

and consequently

$$(k'|t|k) = \frac{2\pi V_0}{\mu v} [(\mu^2 + (k - k')^2)^{-1} + (\mu^2 + (k + k')^2)^{-1}], \quad (B4)$$

where v is the normalization volume for the wave functions. Using this and going over from the summation over k' to an integral by the relation

$$\sum_{k'} \rightarrow \frac{v}{(2\pi)^3} \int dk', \quad (B5)$$

we find

$$\Delta E_3 = \left(\frac{2\pi V_0}{\mu v} \right)^3 v \frac{\mu^{*2}}{(2\pi)^3} \int_{k' > k_F} dk' [(\mu^2 + (k - k')^2)^{-1} + (\mu^2 + (k + k')^2)^{-1}]^2 [\mu^{-2} + (\mu^2 + 4k'^2)^{-1}]$$

$$\times (k^2 - k'^2)^{-2}. \quad (B6)$$

To exhibit the A dependence of this result, we make the rather crude approximation of replacing k by its average value for a Fermi gas, i.e., $k_{Av} = (\frac{3}{5})^{\frac{1}{2}} k_F$ and multiply by the number of pairs $A^2/2$ (for $A \gg 1$). Also, writing $v = (4/3)\pi r_0^3 A$, we find

$$\Delta E_3 = \frac{1}{2} \left(\frac{V_0}{\mu} \right)^3 \left(\frac{4}{3} \pi r_0^3 \right)^{-2} f(k_F), \quad (B7)$$

with $f(k_F)$ independent of A. This integral has been evaluated and gives a value for ΔE_3 of about 10 Mev and thus of 10 Mev/A per particle.