LADC-6291

APR 15 1964

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Localized Green's Functions and Independent-Particle Approximations* for Bound Systems

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ABSTRACT

Localized Green's functions are defined for bound systems. An independent-particle approximation analogous to the Hartree-Fock procedure is derived; the first correction is shown to be identical with that determined in a corresponding shell model. An independent-particle approximation based on use of the free two-particle t matrix instead of the interparticle potential is formulated and its first correction is shown to be similar to that in a suitably constructed shell model.

*Work performed under the auspices of the U. S. Atomic Energy Commission.

DISCLAIMER

Localized Green's Functions

In a previous paper[1], it was shown that the Green's functions for bound systems are

$$G_{N\underset{\sim}{k}}(1\ldots n;1'\ldots n') = (-i)^n\langle g_N\,-\underset{\sim}{k}/2|T\big(\psi(1)\ldots\psi(n)\psi^\dagger(n')\ldots\psi^\dagger(1')\big)|g_N\ \underset{\sim}{k}/2\rangle$$

$$= (-i)^n e^{i\underset{\sim}{k}\cdot\underset{\sim}{A}}\langle g_N\,-\underset{\sim}{k}/2|T\big(\psi(1-A)\ldots\psi(n-A)\psi^\dagger(n'-A)\ldots\psi^\dagger(1'-A)\big)|g_N\ \underset{\sim}{k}/2\rangle \tag{1}$$

Here $1 = x_1 = (t_1, \underset{\sim}{x}_1)$; the state $|g_N\ \underset{\sim}{k}/2\rangle$ is the ground state g_N of the N-particle system with total momentum $\underset{\sim}{k}/2$. The vector A is any four-vector.

The Green's functions of Eq. (1) are not suitable for independent-particle approximation, since the momentum of the state g_N must be conserved. Thus, with the $G_{N\underset{\sim}{k}}$ of (1), one would have to try, for example,

$$G_{N\underset{\sim}{k}}(12;1'2') \approx \int f(\underset{\sim}{k}_1)\ \delta\ (\underset{\sim}{k}_1 + \underset{\sim}{k}_2 - \underset{\sim}{k})\ G_{N\underset{\sim}{k}_1}(1;1')G_{N\underset{\sim}{k}_2}(2;2')d\underset{\sim}{k}_1 d\underset{\sim}{k}_2 \tag{2}$$

as a Hartree approximant. Such an approximant would be difficult to manage because of the integration in (2). Basically, this difficulty is due to the fact that $G_{N\underset{\sim}{k}}$ is not a localized function, while an independent-particle approximation for a bound system presupposes a center for the single-particle orbitals.

In order to obtain a localized Green's function, note first that if A is chosen to be A_c:

$$A_c = \left(\sum x_i + \sum x_i'\right)\Big/ 2n \quad , \tag{3}$$

then the invariant Green's function

$$G^I_{N\underset{\sim}{k}}(1\ldots n;1'\ldots n') = (-i)^n \langle g_N, -\underset{\sim}{k}/2 | T(\psi(1-A_c)\ldots\psi^\dagger(1'-A_c)) | g_N\, \underset{\sim}{k}/2\rangle$$

does not depend on A_c, but only on relative coordinates. However,[2]

$$\begin{aligned} G_N(1\ldots n;1'\ldots n') &\equiv \int d\underset{\sim}{k}\; G_{N\underset{\sim}{k}}(1\ldots n;1'\ldots n') \\ &= \int d\underset{\sim}{k}\; e^{i\underset{\sim}{k}\cdot\underset{\sim}{A}c}\; G^I_{N\underset{\sim}{k}}(1\ldots n;1'\ldots n') \end{aligned} \tag{5}$$

depends on $\underset{\sim}{A}_c$ in an essential way, since G^I depends on $\underset{\sim}{k}$ in an essential way. The localized function G_N is useful also because G^I_N can be obtained from it:

$$G^I_{N\underset{\sim}{k}} = (2\pi)^{-3} \int d\underset{\sim}{A}_c\; e^{-i\underset{\sim}{k}\cdot\underset{\sim}{A}c}\; G_N \quad . \tag{6}$$

Thus G_N contains all the information that G^I does, although Eq. (5) might appear to contradict this. However, it is just that G^I depends on only 2n variables, not 2n + 1; G_N depends on the same number of variables. It does not depend on $\underset{\sim}{k}$, but rather depends in a nontrivial way on all 2n particle coordinates, not just on the relative ones (all this relates to the space coordinates only; the functions all depend

only on relative time coordinates).

As was shown in I, $G_{N\underset{\sim}{k}}$ can be resolved into, for example,

$$G_{N\underset{\sim}{k}}(1;1') = G_o(1;1')\,\delta\,(\underset{\sim}{k}) + G'_{N\underset{\sim}{k}}(1;1') \tag{7}$$

$$G_{N\underset{\sim}{k}}(12;1'2') = G_o(12;1'2')\,\delta\,(\underset{\sim}{k}) + (1 \mp P_{12})(1 \mp P_{1'2'})G_o(1;1')G'_{N\underset{\sim}{k}}(2;2') + G'_{N\underset{\sim}{k}}(12;1'2') \tag{8}$$

Hence, it follows that

$$G_N(1;1') = G_o(1;1') + G'_N(1;1') \tag{9}$$

$$G_N(12;1'2') = G_o(12;1'2') + (1 \mp P_{12})(1 \mp P_{1'2'})G_o(1;1')G'_N(2;2') + G'_N(12;1'2') \tag{10}$$

where

$$G'_N = \int d\underset{\sim}{k}\; G'_{N\underset{\sim}{k}} \tag{11}$$

The differential equations for the functions G_N are obtained by integrating Eqs. (29) and (30) of I:

$$D_1 G_N(1;1') = \delta\,(1-1') \mp i\int V(1-2)G_N(12;1'2^+)\,d2 \tag{12}$$

$$D_1 G_N(1\ldots n;1'\ldots n') = \left(1 \mp \sum_2^{n'} P_{1'i'}\right)\delta\,(1-1')\,G_N(2\ldots n;2'\ldots n') \mp i\int V\Big(1-(n+1)\Big)\,G_N\Big(12\ldots n,n+1;1'\ldots n'(n+1)^+\Big)\,d(n+1) \tag{13}$$

where n^+ stand for $t_n + 0, \underset{\sim}{x}_n$. In terms of the functions G'_N, the

equation for $G_N'(1;1')$ is obtained by integrating I(31):

$$D_1 G_N'(1;1') = \mp i \int V(1\text{-}2) \left[G_o(1;1') G_N'(2;2^+) \mp G_o(2;1') G_N'(1;2^+) + G_N'(12;1'2^+) \right] d2 \quad . \qquad (14)$$

Independent-Particle Approximation

Eq. (10) is fundamental for the discussion of independent-particle approximations. The basic "weak-coupling" approximation that leads to a Hartree-Fock equation is

$$G_N'^{IP}(12;1'2') = G_N'^{IP}(1;1')G_N'^{IP}(2;2') \mp G_N'^{IP}(1;2')G_N'^{IP}(2;1') \tag{15}$$

Note that this approximation by no means requires that the interparticle interaction be weak. Eq. (15) may be a good approximation when

$$G_o(12;1'2') \approx G_o(11')G_o(22') \mp G_o(12')G_o(21') \tag{16}$$

is very bad. This is due to the fact that $G_N'(12;1'2')$ contains only that part of the Green's function in which neither particle propagates freely, nor do both together. If the system is such that once one of the particles interates with g_N it is no longer free to interact independently with the other particle, then (15) can be a good approximation even for strong interparticle interactions. Thus it follows that (15) may be good when

$$G_N(12;1'2') \approx G_N(11')G_N(22') \mp G_N(12')G_N(21') \tag{17}$$

is also quite bad. It is seen that the separation of the free-particle motion that has been made in (10) is important in obtaining a good

independent particle-approximation.

With (15), (14) becomes

$$D_1 G_N'^{IP}(1;1') = \mp i \left(G_o(1;1') + G_N'^{IP}(1;1')\right)\int V(1\text{-}2) G_N'^{IP}(22^+) + i\int \left(G_o(2;1') + G_N'^{IP}(2;1')\right) V(1\text{-}2) G_N'^{IP}(1;2^+) \tag{18}$$

or, with (9)

$$\begin{aligned} D_1 G_N^{IP}(1;1') &= \delta(1\text{-}1') \mp iG_N^{IP}(1;1')\int V(1\text{-}2) G_N'^{IP}(22^+)d2 \\ &\quad + i\int G_N^{IP}(2;1')\, V(1\text{-}2) G_N'^{IP}(1;2^+)d2 \\ &= \delta(1\text{-}1') \mp iG_N^{IP}(1;1')\int V(1\text{-}2) G_N^{IP}(2;2^+)d2 \\ &\quad + i\int G_N^{IP}(2;1')\, V(1\text{-}2) G_N^{IP}(1;2^+)d2 \end{aligned} \tag{19}$$

where

$$G_o(1;2^+)\,\delta\,(t_1 - t_2) = G_o(2;2^+) = 0 \tag{20}$$

has been used.

Equation (19) is just the Hartree-Fock equation in Green's-function form.[3] The interpretation of (19) differs somewhat from the usual one. In the first place, the function G_N in (19) has definite properties

under Galilean transformations. The invariant Green's functions and hence the S matrix can be obtained from G_N via Eq. (6). Secondly, although (19) can be obtained by substituting (17) into (12), it is possible that (19) is a good approximation even when (17) is not, since the derivation of (19) has used only the condition (15), which is weaker than (17). The fact that (15) rather than (17) gives a good independent-particle approximation is a partial explanation of the fact that "strongly" interacting particles like nucleons can be described so well by an independent-particle model.

It is interesting to note that (19) is the limit of another procedure, namely, that in which a central potential $\lambda V(r)$ is assumed to bind the particles around the origin. Then the corresponding Hartree-Fock equation is

$$\left(D_1-\lambda V(1)\right) G_N^{IP}(1;1') = \delta(1-1') \mp iG_N^{IP}(11')\int V(1-2)G_N^{IP}(22^+)d2 + i\int G_N^{IP}(21')V(1-2)G_N^{IP}(12^+)d2 \tag{21}$$

and (19) is the limit of this as $\lambda \to 0$. Thus G_N and not G_{Nk} is obtained by this limiting procedure, and, again, Eq. (6) gives the prescription for obtaining G_{Nk}.

In order to obtain the solutions of (19), it is useful to define the nonlocal Hartree-Fock single-particle potential $W^{IP}(1;1')$ by

$$\int W^{IP}(1,1')f(1')d1' = \mp i \int v(1-2)\left[G_N^{IP}(2;2^+)f(1) \mp G_N^{IP}(1;2^+)f(2)\right] f2 \quad , \qquad (22)$$

where the time-dependence of W^{IP} is given by

$$W^{IP}(1,1') = \delta(t_1 - t_1')\, W^{IP}(\underset{\sim}{x}_1, \underset{\sim}{x}_1') \quad . \qquad (23)$$

With Eq. (22), the equation for $G_N^{IP}(1;1')$ becomes

$$D_1^{IP} G_N^{IP}(1;1') \equiv D_1 G_N^{IP}(1;1') - \int W^{IP}(1,2) G_N^{IP}(2;1')d2 = \delta(1-1') \qquad (24)$$

so that $G_N^{IP}(1;1')$ is just the Green's function for N independent particles in the potential $W^{IP}(\underset{\sim}{x}_1, \underset{\sim}{x}_1')$ and takes the form

$$G_N^{IP}(1;1') = S_\alpha \psi_\alpha(\underset{\sim}{x}_1)\psi_\alpha^*(\underset{\sim}{x}_1')e^{-i\epsilon_\alpha(t_1-t_1')}\, \chi_\alpha(t_1,t_1') \qquad (25)$$

$$\chi_\alpha(tt') = (1 - f_\alpha)\,\theta(t - t') - f_\alpha \theta(t'-t) \qquad (26)$$

Only Fermions are treated from this point on. The analogous treatment for Bosons is easily constructed. Hence, the f_α in (26) are defined by

$$\begin{aligned} f_\alpha &= 1 \qquad \gamma \epsilon O \\ f_\alpha &= 0 \qquad \gamma \notin O \end{aligned} \qquad (27)$$

where O is the set of N single-particle states that are the N lowest eigenstates of

$$-\nabla^2\psi_\alpha(\underset{\sim}{x}) + \int W^{IP}(\underset{\sim}{x},\underset{\sim}{x}')\psi_\alpha(\underset{\sim}{x}')d\underset{\sim}{x}' = \epsilon_\alpha\psi_\alpha(\underset{\sim}{x}) \tag{28}$$

Of course, the potential W is found by a self-consistent procedure, since it must satisfy (23); the latter involves only the "occupied" single-particle states.

It is worth noting that in the Hartree-Fock approximation there is a vector $|HF\rangle$ such that

$$G_N^{IP} = (-i)^n \langle HF|T|HF\rangle \tag{29}$$

where T stands for a time-ordered product. However, it is not true in general that there exists a vector $|\alpha\rangle$ such that the exact Green's functions G_N can be written

$$G_N = (-i)^n \langle \alpha|T|\alpha\rangle \quad , \tag{30}$$

for if (30) were correct, it would follow that

$$|\alpha\rangle\langle\alpha| = \int d\underset{\sim}{k}\,|g_N\,\tfrac{\underset{\sim}{k}}{2}\rangle\langle g_N,\,-\tfrac{\underset{\sim}{k}}{2}| \tag{31}$$

and, hence,

$$\langle g_N\,-\tfrac{\underset{\sim}{k}}{2}|\alpha\rangle\langle\alpha|g_N\,\tfrac{\underset{\sim}{k}}{2}\rangle = \delta(\underset{\sim}{k}-\underset{\sim}{k}') \tag{32}$$

for all $\underset{\sim}{k}$, clearly impossible. The invalidity of (30) is the main argument for working with Green's functions instead of wave functions.

Correlated Independent-Particle Approximation

If the interparticle potential V is singular at small distances, Eqs. (15) and (18) are not a good approximation. In order to obtain a useful independent-particle approximation, consider Eq. (10) in diagrammatic form as shown in Fig. 1. If $\underset{\sim}{x}_1$ and $\underset{\sim}{x}_2$ are close together, V(1-2) times the second graph on the right side of Fig. 1 can give a divergence. In that case, it is natural to regroup the terms in the way shown in Fig. 2, where some of the graphs in the third term in Fig. 1 have been shifted to the second term in Fig. 2. The single-particle function $S_N(1;1')$ is related to $G_N'(1;1')$ by

$$G_N'(1;1') = G_o(1;2)S_N(2;3)G_o(3;1') \quad , \tag{33}$$

where the convention will be that any repeated index is to be integrated, as 2 and 3 in (33). Hence, the resolution corresponding to Fig. 2 is

$$G_N(12;1'2') = G_o(12;1'2') + G_o(12;1'3)S_N(3;4)G_o(4;2') + G_o(12;32')S_N(3;4)G_o(4;1')$$

$$+ G_o(12;34)S_N(34;56)G_o(5;1')G_o(6;2'). \tag{34}$$

In order to evaluate $V(1-2)G(12;1'2^+)$, the relation

$$V(1-2)G_o(12;34) = t(12;56)\left[G_o(5;3)G_o(6;4) - G_o(5;4)G_o(6;3)\right] \tag{35}$$

is required. Equation (35) follows from the properties of the t matrix:

$$G_o(12;34)=G_o(1;3)G_o(2;4)-G_o(1;4)G_o(2;3)$$

$$+G_o(1;5)G_o(2;6)t(56;78)\left[G_o(7;3)G_o(8;4)-G_o(7;4)G_o(8;3)\right] \tag{36}$$

$$t(12;34)=V(1-2)\delta(1-3)\delta(2-4)+iV(1-2)G_o(1;5)G_o(2;6)t(56;34) \tag{37}$$

It follows from Eqs. (34) and (35) that

$$V(1-2)G_N(121'2^+)=\int t(1234)\left[G_o(31')G_o(45)-G_o(41')G_o(35)\right]S_N(56)G_o(62^+)d3d4d5d6$$

$$+\int t(1234)\left[G_o(35)G_o(46)-G_o(45)G_o(36)\right]S_N(5678)G_o(71')G_o(82^+)d3d4d5d6d7d8 \tag{38}$$

where Eq. (20) and

$$t(1234) \propto \delta(t_1 - t_2)\,\delta(t_3 - t_4)\,\theta(t_1 - t_3) \tag{39}$$

have been used. Equation (38) gives

$$D_1G_N(1;1') = \delta(1-1') - i\int t(1234)\left\{G_o(31')G_N'(42^+)-G_o(41')G_N'(32^+)\right.$$

$$\left.+\,G_N''(34;1'2^+)\right\}d2d3d4 \tag{40}$$

where

$$G_N''(34;1'2^+) \equiv \left[G_o(35)G_o(46)-G_o(36)G_o(45)\right]S_N(5678)G_o(71')G_o(82^+) \tag{41}$$

In (40) and (41), $G_N''(34;1'2^+)$ is a two-particle Green's function in which the particles at 3 and 4 are not allowed to interact with each

other without first interacting with the medium. Hence, the correlated independent-particle approximation is

$$G_N''^{ClP}(34;1'2^+) = G_N'^{ClP}(31')G_N'^{ClP}(42^+) - G_N'^{ClP}(32^+)G_N'^{ClP}(41') \qquad (42)$$

and gives

$$D_1 G_N^{ClP}(1;1') = \delta(1-1') - i\int t(1234)\left[G_N^{ClP}(31')G_N^{ClP}(42^+) - G_N^{ClP}(32^+)G_N^{ClP}(41')\right] d2d3d4 \qquad (43)$$

The result given by Eq. (43) is just the Hartree-Fock equation (19) with V replaced by t, the free two-particle t matrix. The t matrix here is not defined self-consistently,[4] although better convergence might be obtained with a self-consistent t. However, the simplicity of (43), together with its resemblance to (19) are attractive features that would be lost by use of a self-consistent two-body t matrix.

Again, (43) has been derived on the assumptions that (19) needs correcting only for $\underset{\sim}{x}_1 - \underset{\sim}{x}_2$ small and that the particles interact freely when they are close together.

Since t(12;34) has times equal in pairs, Eq. (43) can be solved like Eq. (19), namely $W^{ClP}(1,1')$ is defined by

$$-i\int t(12;34)G_N^{ClP}(4;2^+)f(3)d2d3d4 + i\int t(1234)G_N^{ClP}(32^+)f(4)d2d3d4 = \int W^{ClP}(1;1')f(1')d1' \qquad (44)$$

$$W^{\mathrm{ClP}}(1,1') = \frac{1}{2\pi}\int d\omega\, e^{-i\omega(t_1-t_1')} W_\omega^{\mathrm{ClP}}(\underset{\sim}{x}_1\, \underset{\sim}{x}_1') \tag{45}$$

Then Eqs. (25) - (28) and (44), (45) with W^{IP} replaced by $W_{\epsilon_\alpha}^{\mathrm{ClP}}$ specify the solutions of the correlated independent-particle approximation (43).

In this case, the fact that the potential $W_{\epsilon_\alpha}^{\mathrm{ClP}}$ depends on the energy ϵ_α of the single-particle state shows that even in the lowest approximation there is no vector $|\alpha\rangle$ such that G^{ClP} is an expectation value in the state $|\alpha\rangle$ of a time-ordered product.

Corrections to the Independent-Particle Approximation

In order for (19) to be useful, it is necessary to have a systematic procedure for computing the corrections to the independent-particle approximations to the Green's functions. The substitutions

$$G_N(1;1') = G_o(1;1') + G_N'(1;1') \tag{46}$$

$$G_N(12;1'2') = G_o(12;1'2') + (1-P_{12})(1-P_{1'2'})G_o(11')G_N'(22')+G_N'(12;1'2') \tag{47}$$

$$G_N'(12;1'2') = (1-P_{12})G_N'(11')G_N'(22) + K_N(12;1'2') \tag{48}$$

$$\begin{aligned} G_N(123;1'2'3') = G_o(123;1'2'3') &+ \left\{G_o(12;1'2')G_N'(33')\right\} \\ &+ \left\{G_o(11')G_N'(23\ 2'3')\right\} + G_N'(123;1'2'3') \end{aligned} \tag{49}$$

$$G_N'(123;1'2'3') = \left\{G_N'(11')G_N'(22')G_N'(33')\right\}+\left\{G_N'(11')K_N(23\ 2'3')\right\}+ K_N(123;1'2'3') \tag{50}$$

where the curly brackets indicate antisymmetrization in $123;1'2'3'$, in (12) and (13) give, after considerable manipulation,

$$D_1G_N(1;1')=\delta(1-1')-i\int V(1-2)\left[G_N(11')G_N(22^+)-G_N(12^+)G_N(21')+K_N(12;1'2^+)\right]d2 \tag{51}$$

$$\begin{aligned} D_1K_N(12;1'2') = &\\ -i\int V(1-3)\Big[&G_N(33^+)K_N(12;1'2')-G_N(13^+)K_N(32;1'2')+G_N(23^+)G_N(12')G_N(31') \\ &-G_N(23^+)G_N(11')G_N(32')-G_o(23^+)G_o(13;2'1') \end{aligned}$$

$$+G_N(11')K_N(23\ 2'3^+) + G_N(12')K_N(23\ 3^+1')+G_N(23^+)K_N(31;1'2') \qquad (52)$$

$$+G_N(31')K_N(12;2'3^+) + G_N(32')K_N(12;3^+1')+K_N(123;1'2'3^+)$$

$$+G_N(23^+)\Big(G_o(31;1'2')-G_o(12')G_o(31')+G_o(11')G_o(32')\Big)$$

$$+G_N(13^+)\Big(G_o(23;1'2')-G_o(21')G_o(32')+G_o(22')G_o(31')\Big)$$

$$+G_N(33^+)\Big(G_o(12;1'2')-G_o(11')G_o(22')+G_o(12')G_o(21')\Big)\Big]\,d3$$

The equations for $K_N(123;1'2'3')$, etc., can be obtained similarly.

As is readily seen from (51), $K_N(12;1'2^+)$ is a measure of the deviation of $G_N(1;1')$ from $G_N^{IP}(1;1')$; if $K_N(12;1'2')$ is set equal to zero, Eq. (51) becomes the independent-particle equation (19). The function $K_N(12;1'2')$ is thus a sort of two-particle correlation Green's function. There are at least two ways of attacking (51) and (52). The first method will be called the perturbative independent-particle (PIP) method. In this method the self-consistent independent-particle potential W^{IP} and the function $G_N^{IP}(1;1')$ are chosen by the process described in conjunction with Eqs. (22) - (28). Then the expansions

$$G_N(1;1') = G_N^{IP}(1;1') + G_N^{(1)}(1;1') + G_N^{(2)}(1;1') +\cdots \qquad (53)$$

$$K_N(12;1'2') = K_N^{(1)}(12;1'2') + K_N^{(2)}(12;1'2') +\cdots \qquad (54)$$

$$K_N(123;1'2'3') = K_N^{(2)}(123;1'2'3') +\cdots \qquad (55)$$

are substituted into (51) and (52); Eq. (51) can be written

$$D_1^{IP} G_N(1;1') =$$

$$\delta(1-1') - i\int V(1-2)\left[\left(G_N(22^+) - G_N^{IP}(22^+)\right)G_N(11') - \left(G_N(12^+) - G_N^{IP}(12^+)\right)G_N(21') + K_N(12;1'2^+)\right] . \qquad (56)$$

In (56), W^{IP} must be taken to be of zeroth order, so that substitution of (53) and (54) gives first Eq. (24) and then

$$G_N^{(1)}(1;1') = 0 \qquad (57)$$

$$D_1^{IP} G_N^{(2)}(1;1') = -i\int V(1-2) K_N^{(1)}(12;1'2^+)d2 \qquad (58)$$

It should be noted that one of the virtues of the choice of potential prescribed by the independent-particle approximation is that it makes the first correction to $G_N(1;1')$ of second order; this is essentially due to the variational aspect of the Hartree-Fock approximation.

According to (58) the first correction to $G_N^{IP}(1;1')$ is determined by $K_N^{(1)}(12;1'2')$. In Eq. (52), the substitution

$$L_N(12;1'2') = K_N(12;1'2') + G_o(12;1'2') - G_o(11')G_o(22') + G_o(12')G_o(21') \qquad (59)$$

$$= G_N(12;1'2') - G_N(11')G_N(22') + G_N(12')G_N(21')$$

gives

$$D_1^{IP} L_N(12;1'2')$$

$$= -i\int V(1\text{-}2)\Big[\Big(G_N(33^+)-G_N^{IP}(33^+)\Big)L_N(12\ 1'2')-\Big(G_N(13^+)-G_N^{IP}(13^+)\Big)L_N(12\ 1'2') \tag{60}$$

$$+ G_N(23^+)G_N(12')G_N(31')-G_N(23^+)G_N(11')G_N(32')$$

$$+ G_N(11')L_N(23\ 2'3')+G_N(12')L_N(23\ 3^+1')+G_N(23^+)L_N(31\ 1'2')$$

$$+ G_N(31')L_N(12\ 2'3^+)+G_N(32')L_N(12\ 3^+1')+K_N(123;1'2'3^+)\Big]\,d3$$

and, hence,

$$D_1^{IP} L_N^{(1)}(12;1'2')$$

$$= -i\int V(1\text{-}2)G_N^{IP}(23^+)\Big[G_N^{IP}(12')G_N^{IP}(31')-G_N^{IP}(11')G_N^{IP}(32')\Big]\,d3 \tag{61}$$

so that $L_N^{(1)}$ is determined by $G_N^{IP}(1;1')$. Note that (59), substituted into (58), gives

$$D_1^{IP} G_N^{(2)}(1;1') = -i\int V(1\text{-}2)L_N^{(1)}(12;1'2^+)d2 \quad , \tag{62}$$

so that (61) and (62) together give the lowest-order correction to $G_N^{IP}(1;1')$ and the lowest-order approximation to $L_N(12;1'2')$.

It can easily be verified that Eqs. (61) and (62) are the first-order equations of a shell model, namely, that they are the first-order equations for the Green's functions associated with the Hamiltonian

$$H^{IP} = -\int \psi^\dagger(x') \left(\delta(x-x')\nabla^2 - W^{IP}(x',x')\right) \psi(x)dx\,dx' \qquad (63)$$

$$+ \frac{1}{2}\int \psi^\dagger(x)\psi^\dagger(y)v(x-y)\psi(x)\,dx\,dy - \int \psi^\dagger(x)\, W^{IP}(x,x')\, \psi(x')\,dx\,dx'$$

which is just the shell-model associated with the Hartree-Fock single-particle orbitals given by Eq. (28). Hence the PIP method is just the usual perturbation theory based on the zeroth-order functions determined by the Hartree-Fock procedure.

An alternative method to the perturbative independent-particle method is the self-consistent independent-particle (SCIP) method. In this method the single-particle potential $W^{SC}(1,1')$ is defined by

$$-\int V(1-2)\left[G_N(22^+)f(1)-G_N(12^+)f(2)\right] d2 = \int W^{SC}(1'1)f(1')d1' \qquad (64)$$

where $G_N(12^+)$ is the single-particle Green's function <u>to the order of the calculation</u>. Then (51) becomes

$$D_1^{SC}G_N(1;1') \equiv D_1G_N(1;1')-\int W^{SC}(11'')G_N(1''1')d1'' = \delta(1-1')-i\int V(1-2)L_N(12;1'2^+)d2 \qquad (65)$$

and (52) and (59) give

$$D_1^{SC}L_N(12;1'2') \qquad (66)$$

$$= -i\int V(1-2)\Big[G_N(23^+)\Big\{G_N(12')G_N(31')-G_N(11')G_N(32')\Big\}+G_N(11')L_N(23\ 2'3^+)$$

$$+G_N(12')L_N(23;3^+1')+G_N(23^+)L_N(31\ 1'2')+G_N(31')L_N(12\ 2'3^+)$$

$$+G_N(32')L_N(123^+1')+K_N(123;1'2'3^+)\Big]\,d3 \quad .$$

In first order, the SCIP method gives

$$D_1^{SC}L_N^{(1)}(12;1'2') \tag{67}$$

$$= -i\int V(1\text{-}2)G_N(23^+)\Big[G_N(12')G_N(31')-G_N(11')G_N(32')\Big]\,d3 \quad ,$$

and (65) and (64); these three equations must be solved self-consistently.

A possible advantage of the SCIP method over the PIP method is in the treatment of situations where collective effects appear. For example, an asymmetric W(11") can appear in the SCIP method more easily than in the PIP method, since it is to a large extent the "residual" interparticle interaction (that is, not included in W^{IP}) that is responsible. Similarly, the SCIP method might be expected to be better than the PIP method in cases where pairing forces are strong.

Corrections to the Correlated Independent-Particle Approximation

The exact equation for the single-particle Green's function is Eq. (40). Instead of (42), the equation

$$G_N''(12;34) = G_N'(13)G_N'(24) - G_N'(14)G_N'(23) + J_N(12;34) \tag{68}$$

must be used. The analog of (43) and (51) is

$$D_1 G_N(1;1') = \delta(1-1') - i\int t(1234)\left[G_N(31')G_N(42^+) - G_N(32^+)G_N(41') + J_N(34\ 1'2^+)\right] d2d3d4 \tag{69}$$

The function J_N is a measure of the deviation of $G_N(1;1')$ from $G_N^{CIP}(1;1')$. If $J_N = 0$, then $G_N = G_N^{CIP}$. In order to obtain an equation for $J_N(1234)$, it is necessary to use expressions for $G_N(123\ 1'2'3')$ analogous to (34) and illustrated in Fig. 3:

$$\begin{aligned} G_N(123\ 1'2'3') &= G_o(123\ 1'2'3') + G_o(123\ 1'2'4')S_N(45)G_o(53') \\ &+ G_o(123\ 1'43')S_N(45)G_o(52') + G_o(123\ 42'3')S_N(45)G_o(51') \\ &+ G_o(123\ 1'45)S_N(4567)G_o(62')G_o(73') + G_o(123\ 42'5)S_N(4567)G_o(61')G_o(73') \\ &+ G_o(123\ 453')S_N(4567)G_o(61')G_o(72') \\ &+ G_o(123\ 456)S_N(456\ 789)\ G_o(71')G_o(82')G_o(93') \quad . \end{aligned} \tag{70}$$

Since

$$\delta(t_1-t_3)G_o(123\ 1'2'3^+) = G_o(23^+)G_o(31\ 1'2') \tag{71}$$

if follows that

$$V(1-3)G_o(123\ 1'2'3^+)=G_o(23^+)\int t(1345)\left[G_o(42')G_o(51')-G_o(41')G_o(52')\right]d4d5 \tag{72}$$

can be used with four of the terms in (70). For the others it is necessary to consider the structure of $G_o(123\ 1'2'3')$. Since a perturbation theory in t is the result that is sought, it is useful to write $G_o(123\ 1'2'3')$ in the form (Fig. 4):

$$\begin{aligned} G_o(123\ 1'2'3') = {} & A'\left[G_o(11')G_o(22')G_o(33')\right] \\ & + A'\left[G_o(11')G_o(24)G_o(35)t(4567)G_o(62')G_o(73')\right. \\ & \quad +G_o(22')G_o(14)G_o(35)t(4567)G_o(61')G_o(73') \\ & \quad \left.+G_o(33')G_o(14)G_o(25)t(4567)G_o(61')G_o(72;)\right] \\ & + A'\left[G_o(14)G_o(25)G_o(36)T(456\ 789)G_o(71')G_o(82')G_o(93')\right] \end{aligned} \tag{73}$$

where A' is the antisymmetrization operator in the coordinates 1',2',3'. A study of the diagram structure of (73), together with Eq. (37) gives

$$\begin{aligned} V(1-3)G_o(123;1'2'3') = {} & A'\left[G_o(22')t(1345)G_o(41')G_o(53')\right] \\ & +A'\left[G_o(24)T(143;567)G_o(51')G_o(62')G_o(73')\right] \end{aligned} \tag{74}$$

and, also, the integral equation for T itself:

$$T(123\ 1'2'3') = \sum_{i=1}^{3} T_i(123\ 1'2'3') \tag{75}$$

$$T_2(123;1'2'3') = T_1(231;2'3'1') = T_3(312;3'1'2') \tag{76}$$

$$\begin{aligned} T_1(123;1'2'3') = {} & t(12;1'4)G_0(44')t(4'3;2'3')+t(1242')G_0(44')t(4'3;1'3') \\ & + t(1245)G_0(44')G_0(55')\left[T_2(4'5'3;1'2'3')+T_3(4'5'3;1'2'3')\right] \end{aligned} \tag{77}$$

Equation (77) can be regarded as the basic integral equation for determining the properties of the free three-particle system from the free two-particle t matrix. It is clear from the iterative treatment of (77) that T itself is of second and higher order in the two-particle t matrix.

In addition, $J_N(123;1'2'3')$ is defined by

$$\begin{aligned} G_N''(123;1'2'3') &= A'\left[G_0(14)G_0(25)G_0(36)S_N(456\ 789)G_0(71')G_0(82')G_0(93')\right] \\ &= \left\{G_N'(11')G_N'(22')G_N'(33')\right\}+\left\{G_N'(11')J_N(23\ 2'3')\right\} \\ &\quad + J_N(123;1'2'3') \ . \end{aligned} \tag{78}$$

After considerable manipulation, the equation for $J_N(12;1'2')$ is found to be

$$\begin{aligned} D_1 J_N(121'2') = -i\int t(1345)\Big\{ & G_N(53^+)\ J_N(42;1'2')-G_N(43^+)J_N(52;1'2') \\ & +G_N(23^+)\left[G_N(42')G_N(51')-G_N(41')G_N(52')\right]+J_N(45\ 1'2') \end{aligned} \tag{79}$$

$$-G_o(23^+)\Big[G_N(42')G_N(51')-G_N(41')G_N(52')-G_N'(42')G_N'(51')+G_N'(41')G_N(52')\Big]$$

$$+G_N(61')J_N(272'3^+) + G_N(62')J_N(72\ 1'3^+)$$

$$+G_N(71')J_N(622'3^+)+G_N(72')J_N(26\ 1'3^+)+J_N(627\ 1'2'3^+)\Big\} \quad .$$

In Eqs. (69) and (79), the preturbative expansions

$$G_N(1;1') = G_N^{CIP}(1;1')+G_N^{(1)}(1;1')+G_N^{(2)}(1;1')+ \cdots \tag{80}$$

$$J_N(12;1'2') = J_N^{(1)}(12;1'2')+J_N^{(2)}(12;1'2')+\cdots \tag{81}$$

$$J_N(123;1'2'3') = J_N^{(2)}(123;1'2'3')+\cdots \tag{82}$$

give Eq. (43) for $G_N^{CIP}(1;1')$ and

$$G_N^{(1)}(1;1') = 0$$

$$D_1^{CIP}G_N^{(2)}(1;1')$$

$$\equiv D_1G_N^{(2)}(1;1')-\int W^{CIP}(1;1")G_N^{(2)}(1";1')d1"=-i\int t(1234)J_N^{(1)}(341'2^+)d2d3d4 \tag{84}$$

$$D_1^{CIP}J_N^{(1)}(12;1'2')$$

$$= -i\int t(1345)\Big\{G_N^{CIP}(23^+)\Big[G_N^{CIP}(42')G_N^{CIP}(51')-G_N^{CIP}(41')G_N^{CIP}(52')\Big]$$

$$-G_o(23^+)\Big[G_N^{CIP}(42')G_N^{CIP}(51')-G_N^{CIP}(41')G_N^{CIP}(52') \tag{85}$$

$$-G_N'^{CIP}(42')G_N'^{CIP}(51')+G_N'^{CIP}(41')G_N'^{CIP}(52')\Big]\Big\} \quad .$$

In Eq. (84), $J_N^{(1)}(34\ 1'2^+)$ only occurs for $t_3 = t_4$; it follows that for $t_1 = t_2$, the term in (85) with factor $G_o(23^+)$ is zero. Hence, the first correction $G_N^{(2)}(1;1')$ is of second order in t and is similar to the correction in a shell model with $G_N^{CIP}(1;1')$ the Green's function describing the "noninteracting" particles in their orbitals and with interparticle interaction given by t. Since the single-particle orbitals are not orthogonal, it is not possible to write a Hamiltonian for this equivalent shell model in configuration space, although in the space with nonorthogonal basis $\varphi_\epsilon(x)$, the Hamiltonian is

$$H^{CIP} = \sum \epsilon\, a_\epsilon^\dagger a_\epsilon + \frac{1}{2}\sum (\alpha\beta|t|\gamma\delta) a_\alpha^\dagger a_\beta^\dagger a_\delta a_\gamma - \sum (\alpha|w^{CIP}|\beta) a_\alpha^+ a_\beta$$

$$\left\{a_\sigma,\ a_\tau^\dagger\right\} = \delta_{\sigma\tau} \tag{86}$$

$$\left\{a_\sigma,\ a_\tau\right\} = 0 \quad .$$

In this case, the equations for the Green's functions are not identical with those in the shell model given by (86). The perturbation theory based on the zeroth-order given by the correlated-independent-particle approximation is most easily carried out by using Green's functions.

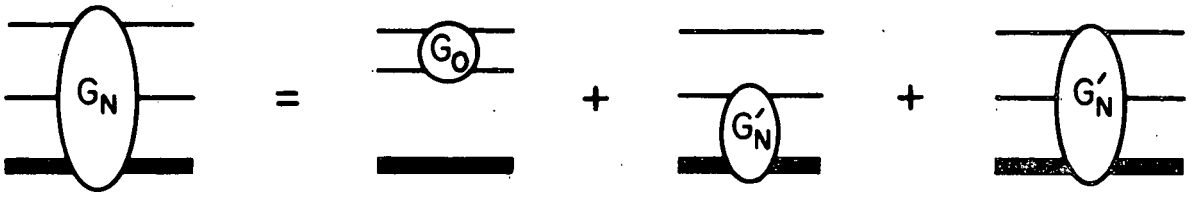

Figure 1 - Equation (10) in diagrammatic form.

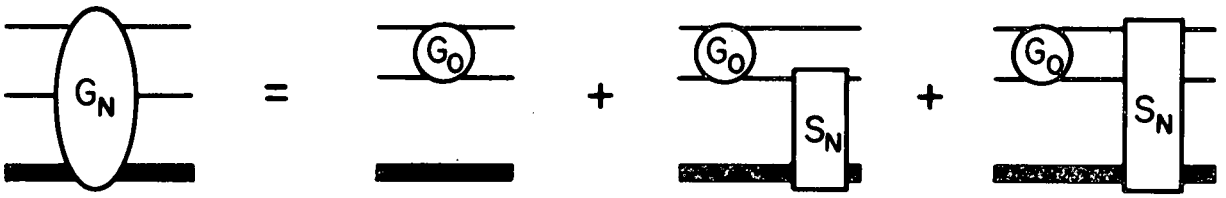

Figure 2 - Equation (34) in diagrammatic form.

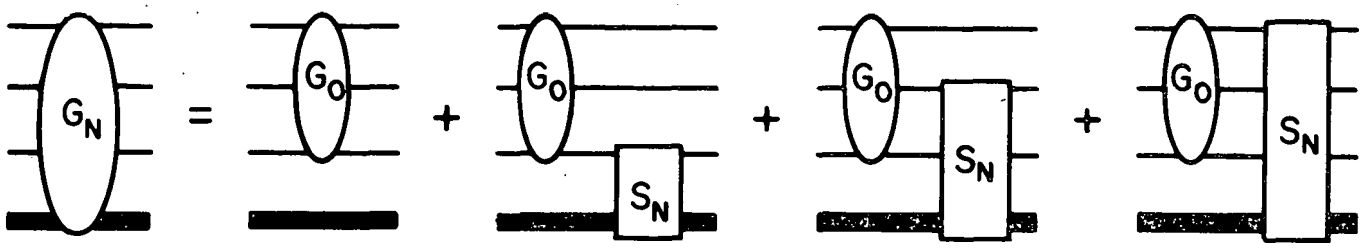

Figure 3 - Resolution of three-particle Green's function.

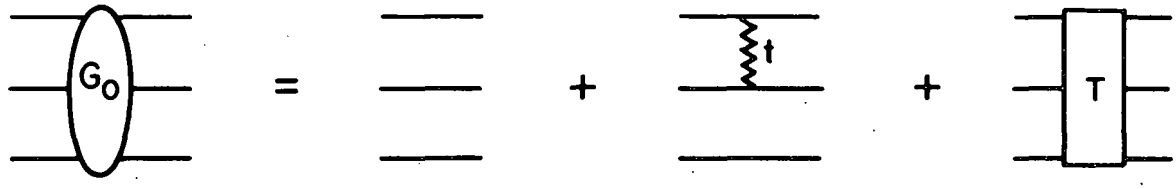

Figure 4 - Resolution of the free three-particle Green's function.

[1] M. Bolsterli, submitted to Phys. Rev.

[2] M. Bolsterli, Bull. Am. Phys. Soc. 7, 611 (1962).

[3] See, for example, L. P. Kadanoff and G. Baym, Quantum Statistical Mechanics (W. A. Benjamin, Inc., New York, 1962).

[4] See the discussion of Brueckner Theory in D. J. Thouless, The Quantum Mechanics of Many-Body Systems (Academic Press, New York, 1961).