portion of Fig. 9. If all the perturbations are small enough, so that no large changes in the eigenvectors are induced, the effective F^{19} hyperfine interaction for CoF approximates that for CoF_2 as follows. Denote the states for CoF_2 in an uncoupled representation $|M_S M_{Co} M_{F1} M_{F2}\rangle$,[44] and consider, for example, the states with $M_{Co}=-\frac{5}{2}$. Then $|\frac{1}{2}-\frac{5}{2}-\frac{1}{2}-\frac{1}{2}\rangle$ is perturbed both by $|\frac{1}{2}-\frac{7}{2}\frac{1}{2}-\frac{1}{2}\rangle$ and by $|\frac{1}{2}-\frac{7}{2}-\frac{1}{2}\frac{1}{2}\rangle$ by the same amount as $|\frac{1}{2}-\frac{5}{2}-\frac{1}{2}\rangle$ is perturbed by $|\frac{1}{2}-\frac{7}{2}\frac{1}{2}\rangle$ because the energy denominators as well as the matrix elements are the same for CoF_2 as for CoF. Also, since both $|\frac{1}{2}-\frac{5}{2}-\frac{1}{2}\frac{1}{2}\rangle$ and $|\frac{1}{2}-\frac{5}{2}\frac{1}{2}-\frac{1}{2}\rangle$ suffer the same perturbation from $|\frac{1}{2}-\frac{7}{2}\frac{1}{2}\frac{1}{2}\rangle$, their degeneracy is not split, but the levels are shifted only half as far as $|\frac{1}{2}-\frac{5}{2}-\frac{1}{2}-\frac{1}{2}\rangle$. So the perturbations do not disturb either statistical intensities or the relative spacings in the group of lines for any M_{Co}, but the hyperfine spacing changes from the first-order perturbation prediction. All the perturbations indicated in Fig. 9, and the smaller ones not indicated, are additive. Therefore, to a good approximation, fluorine hyperfine separations calculated by diagonalizing the 32×32 Hamiltonian for CoF may be transferred to the spectrum of CoF_2, and, by the same argument, to the Hamiltonian [Eq. (1)] for $(CoF_6)^{4-}$.

[44] In this paragraph, eigenkets with three quantum numbers belong to the CoF problem; those with four quantum numbers to the CoF_2 problem.

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Approximation Methods in Many-Body Perturbation Theory*

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An analysis of some approximations common in the treatment of many-body systems indicates that the inclusion of large numbers of uncancelled exclusion-principle-violating (EPV) processes leads to meaningless results. We therefore propose as a criterion for the validity of many-body approximations that there should be no such large-scale inclusion of EPV processes. The graphs generated in the BCS theory are analyzed from this point of view.

INTRODUCTION

In a recent paper, Fukushima and Fukuda[1] attempt to calculate the ground state of the BCS (Bardeen, Cooper, Schrieffer) reduced Hamiltonian in the strong-coupling limit by summing a subset of the totality of graphs generated by this Hamiltonian. The graphs chosen—ladder graphs—seem to dominate all others since they are of order Ω^0 whereas the neglected graphs are of order Ω^{-1} or lower. (The volume of the system is Ω.) As the ground-state energy of this system is known, it is possible to determine that the accuracy of their result is very poor and, what is worse, the asymptotic behavior of such functions as the vacuum expectation value of the U matrix is entirely incorrect. Since the subset of connected graphs chosen is a common one, and since its choice in their case seems particularly well justified, it seemed worthwhile to attempt to seek out the source of the difficulty. We state our conclusions in the language of the strong-coupling model although some are valid in general.

In the first part we summarize and analyze some of the results of Fukushima and Fukuda. This leads us to propose in Part II a criterion for the validity of many-body approximations. The third part contains an analysis of the BCS reduced Hamiltonian according to the proposed criterion.

I. THE LADDER APPROXIMATION

In the strong-coupling limit the kinetic-energy operator is replaced by its constant expectation value T. For convenience this constant is set equal to zero by a shift in the zero of the energy. The BCS reduced Hamiltonian in this limit is then

$$H=T+H_1=V\sum_{kk'}c_{k\uparrow}{}^{\dagger}c_{-k\downarrow}{}^{\dagger}C_{-k'\downarrow}C_{k'\uparrow}, \qquad (1.1)$$

where the sums over momenta are limited to a narrow shell around the Fermi surface. One of the authors has analyzed such strongly coupled systems for a general interaction[2]; some of the results are given below for reference.

The vacuum expectation value of the resolvent operator $R(z)$, where z is a complex variable, can be

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[1] K. Fukushima and N. Fukuda, Progr. Theoret. Phys. (Kyoto) 28, 809 (1962).

[2] L. N. Cooper, Phys. Rev. 122, 1021 (1961).

expanded in a power series in V:

$$\langle 0|R(z)|0\rangle=\left\langle 0\left|\frac{1}{H_1-z}\right|0\right\rangle$$
$$=-\frac{1}{z}\sum_{n=0}^{\infty}\left(\frac{1}{z}\right)^n\langle 0|H_1{}^n|0\rangle. \quad (1.2)$$

The vacuum state $|0\rangle$ is defined as the state in which half of the available unperturbed levels are occupied from the bottom; the total number of levels of both spins is assumed to be $4N$, $2N$ being the total number of particles. The above series has a nonzero radius of convergence if the spectrum is bounded above and below.

Using S_n to denote the sum over all connected vacuum to vacuum graphs of order n, $\langle 0|H_1{}^n|0\rangle$ can be decomposed into products of connected graphs as follows:

$$\langle 0|H_1{}^n|0\rangle=V^n[S_n+\sum_{\alpha+\beta=n}C_{\alpha\beta}{}^nS_\alpha S_\beta$$
$$+\sum_{\alpha+\beta+\gamma=n}C_{\alpha\beta\gamma}{}^nS_\alpha S_\beta S_\gamma+\cdots$$
$$+C_{1\ldots1}{}^n(S_1)^n], \quad (1.3)$$

where

$$C_{\alpha_1\cdots\alpha_s}{}^n=\frac{1}{s!}\frac{n!}{\alpha_1!\alpha_2!\cdots\alpha_s!}.$$

A U matrix can then be defined such that

$$U(-it)=\exp(-H_1t). \quad (1.4)$$

It follows that

$$\langle 0|U(-it)|0\rangle=\sum_m|\langle 0|m\rangle|^2e^{-E_mt}$$
$$=\exp[B_0(-Vt)], \quad (1.5)$$

where

$$B_0(-Vt)=\sum_{n=1}^{\infty}\frac{S_n}{n!}(-Vt)^n, \quad (1.6)$$

and $\langle 0|m\rangle$ is the matrix element between the "unperturbed" vacuum and the mth eigenstate of the exact Hamiltonian. The asymptotic behavior of $B_0(-Vt)$ must be dominated by a term linear in t, as $t\to\infty$

$$B_0(-Vt)\sim -\alpha t,$$

where α is the lowest eigenvalue of H.

Fukushima and Fukuda (FF) have chosen to approximate S_n by the sum of all ladder graphs resulting from (1.1), neglecting all other contributions since they are at most of order Ω^{-1}. The sum over all these connected ladder graphs of order n is

$$S_n{}^{\mathrm{FF}}=(n-1)!N^n. \quad (1.7)$$

Inserting this into (1.6) they find that

$$B_0(-Vt)=-\ln(1+NVt). \quad (1.8)$$

This gives an incorrect ground state for attractive potentials and displays the wrong asymptotic behavior; thus the answer has been completely distorted by the approximation.

We observe first that using their approximation for S_n and the decomposition (1.3), gives the inequality

$$|\langle 0|H_1{}^n|0\rangle|_{\mathrm{FF\ approx.}}>|V|^nS_n{}^{\mathrm{FF}}$$
$$=(N|V|)^n(n-1)!. \quad (1.9)$$

On the other hand we have in general

$$\langle 0|H_1{}^n|0\rangle=\langle 0|[V\sum_{kk'}C_{k\uparrow}{}^\dagger C_{-k\downarrow}{}^\dagger C_{-k'\downarrow}C_{k'\uparrow}]^n|0\rangle$$
$$=V^n\sum_{\substack{k_1\cdots k_n\\k_1'\cdots k_n'}}\langle 0|C_{k_1\uparrow}{}^\dagger C_{-k_1\downarrow}{}^\dagger C_{-k_1'\downarrow}C_{k_1'\uparrow}\cdots$$
$$C_{k_n'\uparrow}|0\rangle. \quad (1.10)$$

Further, the vacuum expectation value of products of fermion operators satisfies the inequality

$$|\langle 0|\cdots C\cdots C^\dagger\cdots|0\rangle|\leq 1. \quad (1.11)$$

Such vacuum expectation values will usually be zero. In any case we may write

$$|\langle 0|H_1{}^n|0\rangle|\leq|V^n|\sum_{\substack{k_1\cdots k_n\\k_1'\cdots k_n'}}1=4^n|V|^nN^{2n}. \quad (1.12)$$

The introduction of a similar upper limit was essential in the proof[2] that the expansion of $\langle R(z)\rangle_{ij}$ in powers of the coupling constant has a finite radius of convergence. If one compares Fukushima and Fukuda's result with this upper limit we see that for higher order terms

$$|\langle 0|H_1{}^n|0\rangle|_{\mathrm{FF\ approx.}}>4^n|V|^nN^{2n}, \quad (1.13)$$

which means that the subset of graphs they have selected in their approximation does not correspond to an actual Hamiltonian.

A somewhat closer look at the diagrammatic analysis reveals what is wrong. The evaluation of $\langle 0|H_1{}^n|0\rangle$ by means of Wick's theorem[3] makes it necessary to carry out summations over indices attached to the intermediate particle or hole lines disregarding the restriction imposed by the exclusion principle. We are therefore obliged to include a large number of processes apparently violating this principle so that the violation may

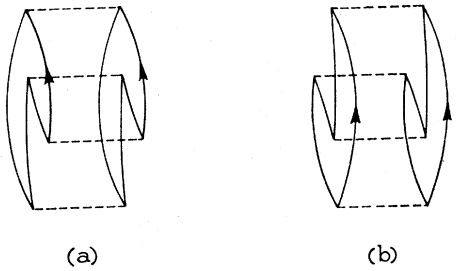


FIG. 1. Some fourth-order graphs which may violate the exclusion principle in intermediate states.

[3] G. C. Wick, Phys. Rev. **80**, 268 (1950).

be cancelled out as a whole. This point has been stressed by Goldstone[4] as extremely important if the linked-cluster expansion is used.

In the fourth order, for example, we see that the graphs shown in Fig. 1, which are included in S_4^{FF} may violate the Pauli exclusion principle in the intermediate states. However, since all the graphs included in S_n^{FF} are positive there is no possible way they can be cancelled. A diagram that contributes to the wanted cancellation, Fig. 2, is neglected in their approximation. This diagram gives a contribution $-N^3$ compared with N^4 for a ladder diagram, but the number of this type increases rapidly with n. This is probably most easily seen as follows. The number of ladder graphs that may violate statistics in intermediate states is $(n-1)!-2^{n-2}$, a rapidly increasing number. For each of these there will usually be several nonladder graphs of opposite sign, all adding up to a contribution which cannot be neglected.

This is however not the only way the exclusion principle can be violated. Following Katz[5] and Mehta,[6] the ladder graphs may be divided into the following

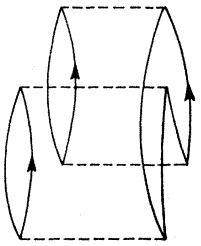


FIG. 2. One of the graphs neglected by Fukushima and Fukuda which contributes to the cancellation of EPV processes contributed by the graphs in Fig. 1.

subgroups; ascending, descending, mixed, and generalized ladder graphs. An example of the ascending ladder graphs which represent only particle-particle scattering, is shown in Fig. 3. These graphs never violate statistics in intermediate states. Suppose now we made the rough approximation of setting S_n equal to the ascending ladder graph. We then obtain

$$S_n^{\text{ascending ladder}}=N^n, \tag{1.14}$$

which leads to

$$B_0(-Vt)=e^{-NVt}-1, \tag{1.15}$$

a result which is (if a comparison can be made) even worse than (1.8).

The reason for this is that the formula (1.3) counts combinations of disconnected graphs such as shown in Fig. 4. One here counts a disconnected graph violating statistics and neglects the connected graphs which in a proper treatment would cancel the violation. As the order n increases, the number of combinations of this type grows rapidly and again can no longer be neglected.

[4] J. Goldstone, Proc. Roy. Soc. (London) **A239**, 267 (1957).
[5] A. Katz, Nucl. Phys. **20**, 663 (1960).
[6] M. L. Mehta, Nucl. Phys. **20**, 533 (1960).

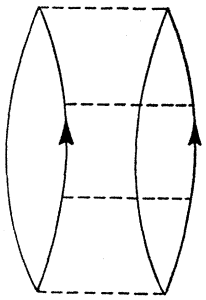


FIG. 3. The fourth-order ascending ladder graph.

II. A CRITERION FOR THE VALIDITY OF MANY-BODY APPROXIMATIONS

The results obtained above show that the difficulties encountered by Fukushima and Fukuda arise from the inclusion of a very large number of exclusion-principle-violating (following Kelly,[7] hereafter abbreviated EPV) processes in higher order terms of the expansion. This suggests further that any approximation used in many-body systems which leads to the inclusion of large numbers of EPV processes, in the absence of evidence to the contrary, should be regarded with suspicion. We are thus led to propose a new criterion for the validity of approximations in many-body systems.

The energy levels (and in particular the ground-state energy of many-body systems) can be obtained from the vacuum expectation value of the U matrix. Now $\langle 0|U(-it)|0\rangle$ contains no contributions from EPV processes. This is meant in the following sense. The anticommutation properties of C and $C^\dagger$ guarantee that any process which violates the Pauli exclusion principle will be exactly cancelled *if all of the graphs are included.*

In order actually to calculate anything one usually makes some approximation to S_n, based possibly on a parameter which is small. Let us call such an approximation $S_n^{(0)}$ where it is understood that $S_n^{(0)}$ is a sum over a subset of the graphs contained in S_n.

$$S_n^{(0)}\subset S_n. \tag{2.1}$$

To obtain information from $S_n^{(0)}$ (e.g., energy levels)

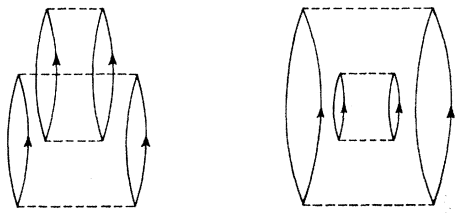


FIG. 4. Some of the fourth-order disconnected graphs composed of connected ascending ladder graphs. These disconnected graphs contain contributions due to processes which violate the exclusion principle.

[7] H. P. Kelly, Phys. Rev. **131**, 684 (1963).

these are recombined as in (1.5) to give an approximated form of $\langle 0|U(-it)|0\rangle$

$$\langle 0|U(-it)|0\rangle^{(0)} \equiv \exp[B_0^{(0)}(-Vt)], \quad (2.2)$$

where

$$B_0^{(0)}(-Vt) \equiv \sum_{n=1}^{\infty} \frac{S_n^{(0)}}{n!}(-Vt)^n. \quad (2.3)$$

However, in doing this the higher order combinations of $S_n^{(0)}$ (to form disconnected graphs) include large numbers of EPV processes—so large that often no recognizable results are obtained. (Our experiments, in addition to those in the previous section, with commonly chosen subsets such as ascending, descending, and mixed ladder graphs in various soluble models yield a wide variety of results bearing little relation to the correct solutions.) The difficulty occurs because we write $\langle 0|U(-it)|0\rangle^{(0)}$ as the *same* function of the approximated set of connected graphs $\{S_1^{(0)}S_2^{(0)}\cdots\}$, as the original $\langle 0|U(-it)|0\rangle$ of the exact set $\{S_1S_2\cdots\}$.

We are therefore led to define a new function

$$\langle 0|U(-it)|0\rangle_{\mathrm{EP}}^{(0)} \equiv \exp\left[\sum_{n=1}^{\infty} \frac{S_n^{(0)}}{n!}(-Vt)^n\right] - [\text{contribution from all EPV processes}]. \quad (2.4)$$

The subscript EP indicates that the new function contains no EPV processes. We note that $\langle 0|U(-it)|0\rangle_{\mathrm{EP}}^{(0)}$ becomes $\langle 0|U(-it)|0\rangle$ when $S_n^{(0)}$ becomes S_n, since for the exact set S_n no EPV processes contribute to the final result. In that case the subtracted term [ ] in (2.4) is zero.

This function is of course harder to calculate than the original, but we propose that it is the function one should at least attempt to calculate. If there is a choice, it seems preferable to exclude from an approximation terms which are not present in the exact result, just as it usually seems preferable to preserve exact symmetries in each order of an approximation.

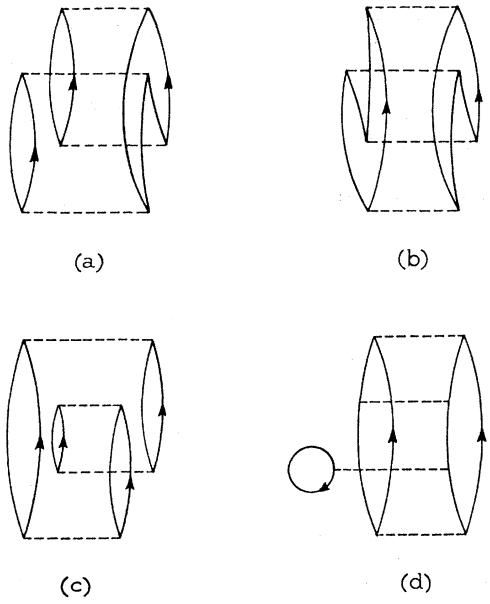


FIG. 5. Some fourth-order EPV graphs. Contributions from graphs (a) and (d) are $-N^3$ and from graphs (b) and (c) N^2.

If we now adopt the attitude that a reasonable subset of the connected graphs (that is one, for example, which is characterized by an expansion in some small parameter) will give us a good approximation if it is inserted in the new function defined above (2.4), the problem becomes to devise a method for calculating this function. One method of obtaining $\langle 0|U(-it)|0\rangle_{\mathrm{EP}}^{(0)}$ from the set $\{S_n^{(0)}\}$, is described below.

Suppose we are given the set of graphs $\{S_n^{(0)}\}$. Let us add to this another set $\{S_n^{(1)}\}$. We require that $\{S_n^{(1)}\}$ has the following properties:

(a) Every process represented by these graphs violates the exclusion principle.

(b) The result obtained when the sum $\{S_n^{(0)}+S_n^{(1)}\}$ is inserted into (2.2) and (2.3) contains no EPV processes.

It then follows that

$$\exp\left[\sum_{n=1}^{\infty} \frac{S_n^{(0)}+S_n^{(1)}}{n!}(-Vt)^n\right] = \langle 0|U(-it)|0\rangle_{\mathrm{EP}}^{(0)}. \quad (2.5)$$

This means that we can calculate in the usual manner with the new set of graphs. We call the set $\{S_n^{(1)}\}$ the proper completion of $\{S_n^{(0)}\}$. In the strong-coupling limit the proper completion, if it exists, is unique.

We are led then, having chosen $\{S_n^{(0)}\}$ possibly on the basis of a small parameter, to add to this a subset $\{S_n^{(1)}\}$ as defined by (2.5) with no reference to this parameter. When this is done the properly completed subset $\{S_n^{(0)}+S_n^{(1)}\}$ will yield a U matrix by the usual formula (1.5).

Any set of connected graphs generated by a Hamiltonian (no matter how truncated) will have the property of yielding a U matrix which contains no EPV processes. Thus we may view the process of proper completion as a process which converts an arbitrary set of graphs into one which might come from a Hamiltonian. Though there is no guarantee that the process can always be carried out, the BCS reduced Hamiltonian can, as we will show in the next section, be viewed as resulting from the proper completion of the ladder graphs.

III. ANALYSIS OF THE BCS REDUCED HAMILTONIAN

The graphs generated by the BCS reduced Hamiltonian may be divided into two disjoint sets:

$$\{S_n^{\mathrm{BCS}}\} = \{S_n^{\mathrm{ladder}}\} + \{S_n^{(1)}\}, \quad (3.1)$$

where $\{S_n^{(1)}\}$ is defined by (3.1) as the set of all non-

ladder BCS graphs. In what follows we show that $\{S_n^{(1)}\}$ so defined is the proper completion of $\{S_n^{\text{ladder}}\}$; thus the BCS Hamiltonian may be viewed as resulting from the proper completion of the set of ladder graphs.

To do this we must show that $\{S_n^{(1)}\}$ satisfies the two criteria for a proper completion stated in Sec. II.

The second requirement follows immediately from the fact that the totality of BCS graphs is generated by the BCS reduced Hamiltonian, thus guaranteeing that no contributions from EPV processes occur.

We next show that the graphs $\{S_n^{(1)}\}$ represent only EPV processes. They are thus distinguished from the ladder graphs which only occasionally contain EPV processes. Thus the only role of the nonladder graphs generated by the BCS Hamiltonian is to compensate for violations of statistics. Some fourth-order examples are shown in Fig. 5.

We first discuss graphs which do not necessarily involve scattering processes with zero momentum transfer. It is observed that all graphs start and end with a pair creation and a pair annihilation vertex. If the only other vertices used are particle-particle and hole-hole scattering vertices, we obtain mixed ladder graphs. This group includes ascending and descending ladder graphs plus graphs representing both hole-hole and particle-particle scattering processes. All these graphs have only two particles and two holes with different spin indices in the intermediate states. Hence

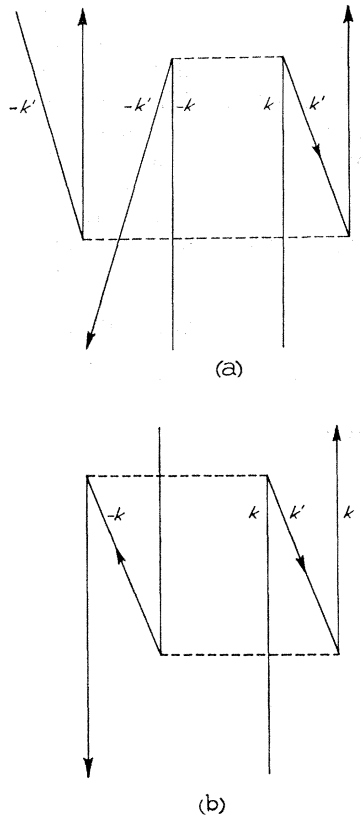


FIG. 6. Exclusion-principle-violating parts of nonladder BCS graphs.

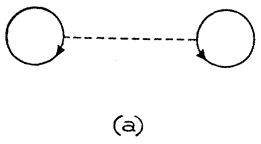
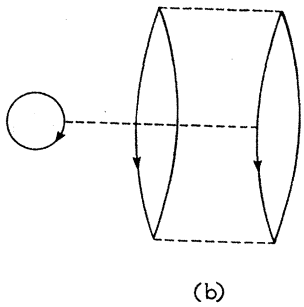


FIG. 7. BCS graphs with bubbles.



these graphs will never violate the Pauli exclusion principle. Other ladder graphs (i.e., some generalized ladder graphs) which are not of this type and nonladder graphs cannot be obtained in this way. In order to find them we must introduce at least one additional pair creation and one pair annihilation vertex. We further notice that if we wish to obtain vacuum to vacuum graphs, these vertices must be introduced in pairs.

A nonladder BCS graph is characterized by the fact that the spin-up and spin-down particle or hole lines are not connected in the same way. A nonladder graph must therefore contain, aside from forward and backward scattering vertices, a pair creation and a pair annihilation vertex connected in one of the ways shown in Fig. 6. Changing the arrow direction in the spin-up part of Fig. 6(a) or reversing the spin-up and spin-down parts give additional possibilities which for the purpose of this discussion are identical to the ones in Fig. 6. Due to the pairing condition, the Pauli exclusion principle is seen to be violated in both these parts. The most general nonladder graph which does not necessarily involve scattering processes with zero momentum transfer, will consist of these parts with particle-particle and hole-hole scattering vertices connected between these two vertices. However this does not alter the fact that these parts of the graph will violate statistics as it is impossible to remove from these parts the repetition of one index by the addition of forward- and backward-scattering vertices.

Scattering processes with zero momentum transfer allow another class of nonladder graphs—those in which a hole line goes back to the same vertex from which it started. Such a part comes from the contractions $[h_{k_i\sigma}h_{k_i\sigma}^{\dagger}]$. Goldstone[4] calls such a loop a passive unexcited particle loop; we will call it a bubble. The sign of a bubble is seen to be positive. Some examples of graphs containing such bubbles are shown in Fig. 7. Some part of these graphs always comes from

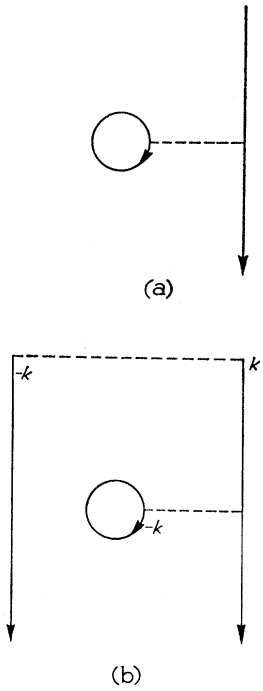


FIG. 8. (a) Characteristic part of a graph containing bubbles. (b) Violation of statistics in this part.

a scattering process with zero momentum transfer. Other graphs, e.g., a descending ladder, may also contain such a process, but this is only for special values of the indices. Excluding the first-order graph, Fig. 7(a), which we may classify as a ladder graph, we see that the characteristic part of such a connected graph is the one drawn in Fig. 8(a). However, the hole line labeled k must also be connected to another hole line labeled $-k$ as shown in Fig. 8(b). We see that this results in a violation of the Pauli exclusion principle. Just as for the previous class of nonladder graphs, it is impossible to remove the repetition of indices by using hole-hole scattering vertices. Hence we may conclude that all nonladder BCS graphs violate statistics. The BCS graphs may therefore be classified as either ladder or EPV graphs. It may be further noted that this is a strict graphical property, which does not depend upon the choice of the strong-coupling model. It will be equally valid if energy denominators were included.

IV. CONCLUSION

Our analysis of the application of various approximations, common in the treatment of many-body systems to the graphs generated by the BCS reduced Hamiltonian, indicates that when used to yield such information as the ground-state energy, large numbers of EPV processes remain uncancelled leading to meaningless results. Since the physical properties of a many-fermion system do not depend upon processes which violate the exclusion principle, if such processes occur (as they do in the usual graphical analysis), they can only play the role of cancelling other EPV processes. We have therefore attempted to arrive at the notion of the "physical graphs" generated by an approximation procedure—those graphs which when combined to produce functions such as $\langle 0|U(-it)|0\rangle$ do not result in any uncancelled EPV processes.

A possible procedure for obtaining these physical graphs from an arbitrary subset of graphs generated through some approximation (based possibly on a small parameter) is proposed. In this one adjoins to the set generated by the approximation another set of graphs called the proper completion. This proper completion, if it exists, is unique and is *not* characterized by the small parameter. Thus the dependence of the total set of graphs on the small parameter is obscured. It is shown that the graphs generated by the BCS reduced Hamiltonian can be regarded as the sum of the ladder graphs and their proper completion.

The easiest method of guaranteeing that a particular set of graphs does not generate any uncancelled EPV contributions and thus does not run into the difficulties we have dealt with is, of course, to generate this set of graphs from a Hamiltonian (no matter how truncated). We observe that two important existing approximate sets of graphs used in the treatment of many-body systems, those used to deal with the long-range part of the Coulomb interaction, and those in the theory of superconductivity can be generated by Hamiltonians.

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