next-nearest-neighbor as well as nearest-neighbor interactions. The ratio of the force constants for these interactions γ/α is related in the model to the compressibility and θ_0 . If we ignore the fact that we are dealing with a hexagonal crystal and calculate this ratio from the present values of κ and θ_0 , it varies between -0.10 to -0.15 depending on the density. It is obvious from the figure that the Debye θ varies much more strongly with temperature than either the other inert gases or the Leighton model with $\gamma/\alpha \sim -0.1$. A comparison with bcc He⁴ and hcp and bcc He³ will be made in another paper but we remark here that the relative temperature dependence of θ in these other forms of solid helium is only very slightly different from that in hcp He⁴.

ACKNOWLEDGMENTS

It is a pleasure to thank Dr. Robert Frost, Edward Ifft, and Peter Seligman for their help in making the measurements, Professor J. G. Daunt for his support and encouragement, and Robert Kindler for his skill in constructing equipment. Professor C. F. Mate kindly read through the manuscript and made valuable suggestions.

PHYSICAL REVIEW

VOLUME 140, NUMBER 3A

1 NOVEMBER 1965

Criteria for the Best Bogoliubov Quasiparticle*

DONALD H. KOBE

Quantum Chemistry Group, Uppsala University, Uppsala, Sweden (Received 26 April 1965; revised manuscript received 16 June 1965)

The principle of compensation of dangerous diagrams has previously been the only general criterion for determining the coefficients in the Bogoliubov canonical transformation to quasiparticles. In this paper it is shown that the criterion of maximum overlap of the true ground state with the BCS ground state gives the same condition for determining the coefficients. The criterion of diagonalizing the quadratic part of the reaction operator, which is a generalization of the Brillouin-Brueckner condition, is also equivalent to the above criteria. Finally these criteria are evaluated from the standpoint of "least labor for the most accuracy."

I. INTRODUCTION

HE problem of treating correlations in many-body systems is always difficult, but one of the most elegant methods is the canonical transformation to quasiparticles introduced by Bogoliubov eighteen years ago. The method was first used by Bogoliubov¹ in treating boson systems,1 and it was successful in obtaining the phonon spectrum. Essentially the same idea was used over a decade later by Bogoliubov² and independently by Valatin³ for fermion systems with attractive interactions to explain superconductivity. In this case the canonical-transformation method gave the energy gap⁴ which was required.

In order to specify the quasiparticles completely, Bogoliubov^{2,5} postulated the principle of compensation

of dangerous diagrams (PCDD) which determined the coefficients in the canonical transformation. A quasiparticle (QP) annihilation operator for fermion systems is defined as²

$$\alpha_1 = u_1 a_1 + v_{-1} a_{-1}^{\dagger}, \qquad (1.1)$$

where a_1 and a_1^{\dagger} are the annihilation and creation operators respectively for a fermion with momentum \mathbf{k}_1 and spin σ_1 and $(1) = (\mathbf{k}_1, \sigma_1)$. They satisfy the usual fermion anticommutation relations. In order for the QP to be fermions also, the coefficients must satisfy the relations

$$u_{1}^{2}+v_{1}^{2}=1,$$

$$u_{1}=u_{-1},$$

$$v_{1}=-v_{-1}.$$
(1.2)

The principle of compensation of dangerous diagrams states that the sum of all diagrams leading from the vacuum to the two QP state is zero. This condition gives an equation from which u_1 and v_1 can be obtained. The justification for postulating the PCDD is that divergences can be removed from the perturbation expansion of the ground-state energy.⁵

In his 1947 paper, Bogoliubov¹ used only the condition of diagonalizing the quadratic part of the Hamil-

^{*} The work reported in this paper has been sponsored in part by the King Gustaf VI Adolf's 70-years Fund for Swedish Culture, Knut and Alice Wallenberg's Foundation, and in part by the Aerospace Research Laboratories, OAR, through the European Office of Aerospace Research (OAR), U. S. Air Force.
¹ N. N. Bogoliubov, J. Phys. (U.S.S.R.) 11, 23 (1947).
² N. N. Bogoliubov, J. h. Eksperim. i Teor. Fiz. 34, 58 (1958) [English transl.: Soviet Phys.—JETP 7, 41 (1958)]; Nuovo Cimento 7, 843 (1958); Usp. Fiz. Nauk 67, 549 (1959) [English transl.: Soviet Phys.—Usp. 2, 236 (1959)].
³ J. G. Valatin, Nuovo Cimento 7, 843 (1958).
⁴ See, e.g., D. H. Douglass, Jr., and L. M. Falicov, in *Progress in Low Temperature Physics*, edited by C. J. Gorter (North-Holland Publishing Company, Amsterdam, 1964), Vol. 4, Chap. III.
⁶ N. N. Bogoliubov, V. V. Tolmachev, and D. V. Shirkov, A

New Method in the Theory of Superconductivity (Academy of Sciences Press, Moscow, 1958) [English transl.: (Consultants Bureau, New York, 1959)]; Fortschr. Physik 6, 605 (1958).

tonian which is the PCDD in lowest order. The PCDD was not enunciated until his work on superconductivity.² For over seven years the PCDD has stood as the general criterion for choosing the coefficients in the canonical transformation. The best method for choosing the coefficients in the transformation of Eq. (1.1) determines the best quasiparticle. The reason that the PCDD has stood so long as the only general criterion is that the second and higher order corrections to it were long considered negligible.⁶ Henley and Wilets⁷ recently showed that the second and higher order corrections are indeed important in the theory of nuclear matter and give results that cannot be obtained from the lowest order term by using perturbation theory. Thus, it is of interest to investigate the foundations of the PCDD to see whether it is firmly established. In order to be more specific, only fermion systems will be considered, but the same ideas can be applied to boson systems as well.

In this paper it will be shown that maximizing the overlap of the exact ground-state vector with the BCS ground-state vector gives exactly the PCDD. Thus, the requirement that the BCS ground state be as close as possible to the true ground state can be taken as the criterion for the best QP. This criterion certainly has a more physically intuitive basis than the mathematical and abstruse PCDD to which it is equivalent. Another criterion for the best QP that is also equivalent to the PCDD is that the quadratic part of the reaction operator be diagonal. The motivation for this work was a paper by Kutzelnigg and Smith⁸ on the foundations of the independent-particle model, where they review many criteria for the best single-particle orbitals.9

The next section gives a review of the PCDD and states it in a precise mathematical form. In Sec. III it will be shown that this form is equivalent to saying that the quadratic part of the reaction operator is diagonal. The equivalence of the PCDD with the maximum overlap of the true ground-state vector and the BCS state vector will be demonstrated in Sec. IV. The criteria will be shown to be compatible with the leastlabor criterion in Sec. V.

II. THE PRINCIPLE OF COMPENSATION OF DANGEROUS DIAGRAMS

Bogoliubov first postulated the principle of compensation of dangerous diagrams to remove divergent terms in the perturbation theory of the ground-state energy.^{2,5} However, just because these divergent terms are re-



FIG. 1. A dangerous contribution to the ground-state energy.

moved does not mean that the perturbation expansion will necessarily converge, or that some other terms might not diverge. The reasons for postulating the PCDD will now be reviewed.

When the usual Hamiltonian for a system of fermions with two-body interactions is transformed to QP by using Eq. (1.1) the result is¹⁰

$$H = \sum_{j+k=0,2,4} H_{jk}, \qquad (2.1)$$

and j, k=0, 1, 2, 3, and 4. The terms in Eq. (2.1) have the form

$$H_{jk} = \sum_{1, \dots, j+k} h_{jk} (1, 2, \dots, j+k) \\ \times \alpha_1^{\dagger} \alpha_2^{\dagger} \cdots \alpha_j^{\dagger} \alpha_{j+1} \cdots \alpha_{j+k}, \quad (2.2)$$

where the coefficients h_{jk} are given in Appendix A of Kobe and Cheston.¹⁰

The true ground state will be called $|0\rangle$ and the state of no QP, i.e., the QP vacuum state, which is the same as the BCS¹¹ ground state, will be called $|\phi_0\rangle$. The true ground-state energy \mathcal{E}_0 can be determined from the Schrödinger equation

$$H|0\rangle = \mathcal{E}_0|0\rangle, \qquad (2.3)$$

by taking the inner product with the BCS ground state, using intermediate normalization $\langle 0 | \phi_0 \rangle = 1$ which gives

$$\mathcal{E}_{0} = H_{00} + \operatorname{Re}\langle\phi_{0}|H_{02}|0\rangle + \operatorname{Re}\langle\phi_{0}|H_{04}|0\rangle. \quad (2.4)$$

The second term on the right is

$$\operatorname{Re}\langle\phi_0|H_{02}|0\rangle = \operatorname{Re}\sum_k h_{02}(k, -k)\langle\phi_0|\alpha_k\alpha_{-k}|0\rangle, \quad (2.5)$$

and vanishes if

$$\operatorname{Re}\langle 0|\alpha_k^{\dagger}\alpha_{-k}^{\dagger}|\phi_0\rangle = 0, \qquad (2.6)$$

since h_{02} is real.¹² This is the condition that Boboliubov^{2,5} has called compensating the dangerous diagrams, and gives an equation from which u_k and v_k can be determined.

In order to see that the second term on the right in Eq. (2.4) can cause divergences, consider the contribution to the ground-state energy shown in Fig. 1. The contribution from Fig. 1 is

$$\mathcal{E}_{0}' = -2 \sum_{\mathbf{k}} \frac{|h_{20}(\mathbf{k}, -\mathbf{k})|^{2}}{2h_{11}(\mathbf{k}, \mathbf{k})},$$

= $-(2\pi)^{-3} \int d\mathbf{k} F(\mathbf{k}),$ (2.7)

⁶ V. V. Tolmachev and S. V. Tiablikov, Zh. Eksperim. i Teor. Fiz. 34, 66 (1958) [English transl.: Soviet Phys.-JETP 7, 46 (1958)

⁷ E. M. Henley and L. Wilets, Phys. Rev. 133, B1118 (1964); Phys. Rev. Letters 11, 326 (1963). I wish to thank the authors for

 ⁸ W. Kutzelnigg and V. H. Smith, Jr., Quantum Chemistry Group, Uppsala, Sweden, Report No. 130, 1964 (unpublished);
 ⁹ J. Chem. Phys. 41, 896 (1964).

⁹ For another point of view on the PCDD see D. H. Kobe, Quantum Chemistry Group, Uppsala, Sweden, Report No. 137, 1964 (unpublished).

¹⁰ See, e.g., D. H. Kobe and W. B. Cheston, Ann. Phys. (N. Y.) 20, 279 (1962). ¹¹ J. Bardeen, L. N. Cooper, and J. R. Schrieffer, Phys. Rev. 108,

^{1175 (1957).}

¹² It also vanishes if $h_{02} = 0$, but this is the PCDD in lowest order which has been shown to be inadequate (see Ref. 7).

where unit volume is assumed. Since the coefficients u_k and v_k are real and satisfy Eq. (1.2), we have the restrictions

$$0 \le u_k \le 1, \tag{2.8}$$

$$0 \leq |v_k| \leq 1.$$

The integrand in Eq. (2.7) is¹³

$$F(\mathbf{k}) = \frac{[2(uv)_k \epsilon_k + (u_k^2 - v_k^2)\Delta_k]^2}{[2(uv)_k \Delta_k + \epsilon_k (u_k^2 - v_k^2)]}, \qquad (2.9)$$

which, of course, can be chosen to be zero. If, however, the conditions

$$2 \ge 2 | (uv)_k| > M_1 \text{ for all } \mathbf{k}$$

$$1 \ge u_k^2 - v_k^2 > M_2 \text{ for } |\mathbf{k}| \text{ sufficiently large }, \quad (2.10)$$

where the M's are constants, are satisfied, then

$$F(\mathbf{k}) \ge \frac{\left[M_{1}\epsilon_{k} + M_{2} | \Delta_{k} | \right]^{2}}{\left[2 | \Delta_{k} | + \epsilon_{k}\right]}$$
(2.11)

if $|\mathbf{k}|$ is sufficiently large. Since $\epsilon_k \sim k^2$ and assuming that $M_4 < |\Delta_k| \leq M_3 k^2$, then \mathcal{E}_0' diverges like k^5 for large values of k.¹⁴ The divergences would be even faster if $|\Delta_k| > M_3 k^2$. Therefore it is best to choose the coefficients u_k and v_k such that $F(\mathbf{k}) = 0$, which means $h_{20}(\mathbf{k},-\mathbf{k})\equiv 0.$

However, Fig. 1 is just one term in the more general diagram shown in Fig. 2. This more general class of diagrams has a contribution which is of the same form as Eq. (2.7), but ϵ_k and Δ_k must be replaced with dressed values $\tilde{\epsilon}_k$ and $\tilde{\Delta}_k$ in one of the h_{20} functions, and the analysis of the last paragraph is still valid. Figure 2 is the set of graphs corresponding to Eq. (2.5) for the ground-state energy.

III. DIAGONALIZING THE QUADRATIC PART OF THE REACTION OPERATOR

The reaction operator t (or t matrix) describes the scattering of particles via a potential V. It is, so to speak, the "dressed" interaction or a pseudopotential which takes into account an infinite number of interactions, since it is obtained from the Lippmann-Schwinger equation¹⁵

$$t = V + VT_0 t. \tag{3.1}$$

In this context the Hamiltonian of Eq. (2.1) has been broken into two parts

$$H = H_0 + V, \qquad (3.2)$$

0 2

FIG. 2. A class of dangerous contributions to the ground-state energy.

¹⁴ This disagrees with a statement made in Ref. 7.
¹⁵ B. A. Lippmann and J. Schwinger, Phys. Rev. 79, 469 (1950).

where

$$H_0 = H_{00} + H_{11}, \qquad (3.3)$$

A 827

and V is the rest of Eq. (2.1). The operator T_0 is defined symbolically as

$$T_{0} = \frac{1 - |\phi_{0}\rangle\langle\phi_{0}|}{\mathcal{E}_{0} - H_{0}}, \qquad (3.4)$$

and is defined more precisely by Löwdin.¹⁶

The reaction operator is in general a many-particle operator. Because of the complicated nature of V in terms of QP, t has an even more complicated nature. In order to specify the QP precisely, i.e., determine the coefficients in the canonical transformation, the quadratic part of t can be diagonalized. This condition gives

$$\operatorname{Re}\langle\phi_0|\alpha_k\alpha_{-k}t|\phi_0\rangle=0,\qquad(3.5)$$

which can be called the Brillouin-Brueckner-Bogoliubov (BBB) condition. It is the natural generalization to QP to the Brillouin-Brueckner condition which says that singly excited configurations do not contribute to the reaction operator.¹⁷ Since a singly excited configuration is the creation of a particle-hole pair, and since a QP is part particle and part hole, the two-QP state is a generalization of the singly excited configuration.

It has been shown that the Brillouin-Brueckner condition can be taken as a basis for the single-particle model, and is essentially equivalent to other criteria for the exact-self-consistent-field approach.⁸ The BBB condition will be shown now to be equivalent to the PCDD. First it will be necessary to define a wave operator W such that it transforms the BCS ground state into the exact ground state

$$|0\rangle = W |\phi_0\rangle. \tag{3.6}$$

The wave operator can be shown to be related to the reaction operator t by¹⁶

$$W = 1 + T_0 t.$$
 (3.7)

Equation (3.5) can be written with the help of Eq. (3.4)as

$$\operatorname{Re}\langle\phi_0|tT_0\alpha_k^{\dagger}\alpha_{-k}^{\dagger}|\phi_0\rangle = 0, \qquad (3.8)$$

since T_0 is acting directly on an eigenstate of H_0 . Using Eqs. (3.6) and (3.7) we obtain

$$\operatorname{Re}\langle 0|\alpha_{k}^{\dagger}\alpha_{-k}^{\dagger}|\phi_{0}\rangle = 0, \qquad (3.9)$$

which is exactly the same as Eq. (2.6). Thus the BBB condition is a necessary and sufficient condition for the PCDD. Equation (3.9) shows that the BBB condition is equivalent to eliminating two QP states from the exact ground state.

¹³ See Ref. 10 for the terms h_{20} and h_{11} .

¹⁶ P. O. Löwdin, J. Math. Phys. 3, 1171 (1962). ¹⁷ L. Brillouin [Actualities Sci. et Ind. No. 71 (1933); No. 159 (1934)] said that $\langle \phi_{aingly} \, excited | V | \phi_0 \rangle = 0$. See also C. Möller and M. S. Plesset, Phys. Rev. 46, 618 (1934). When generalized so that $V \rightarrow t$, it is called the Brillouin-Brueckner condition (Ref. 16). See also R. K. Nesbet, Phys. Rev. 109, 1632 (1958).

IV. MAXIMIZING THE OVERLAP

By far the best criterion for the best Bogoliubov QP is that of maximum overlap of the true ground state with the BCS ground state because it has a more direct physical meaning than the previous two criteria. We can choose the coefficients in the canonical transformation such that the bare QP vacuum or BCS ground state $|\phi_0\rangle$ is as close as possible to the true ground state $|0\rangle$ in Hilbert space, i.e.,

$$\||\phi_0\rangle - |0\rangle\| = \text{minimum}. \tag{4.1}$$

If the norm of the difference between the two states is a minimum, then the overlap between the two states is a maximum

$$X = \operatorname{Re}\langle 0 | \phi_0 \rangle = \operatorname{maximum}. \tag{4.2}$$

This criterion seems to be better than the previous two, since it is not dependent on the behavior of a perturbation expansion or on a rather arbitrary criterion of simplicity. However, Eq. (4.2) will lead back to the PCDD. The maximum overlap criterion for the independent-particle model was first proposed by Brenig.¹⁸

The BCS ground state or QP vacuum state $|\phi_0\rangle$ is defined as the state of no quasiparticles, so for all k

$$\alpha_k |\phi_0\rangle = 0. \tag{4.3}$$

The state vector that satisfies this condition is^{3,11}

$$\phi_0 \rangle = \prod_j (u_j + v_j a_j^{\dagger} a_{-j}^{\dagger}) |\operatorname{vac}\rangle, \qquad (4.4)$$

where $|vac\rangle$ is the state of no particles, and the operator $a_{j}^{\dagger}a_{-j}^{\dagger}$ creates a Cooper pair of particles with equal and opposite momenta and spin. The product in Eq. (4.4) is just over half the total number of states, i.e., $(\mathbf{k}_j)_x \ge 0$, and $|\phi_0\rangle$ is normalized to unity.

The coefficients u_k and v_k in the canonical transformation of Eq. (1.1) satisfy the conditions in Eq. (1.2). In order to maximize the overlap treating u_k and v_k as independent, it is necessary to introduce the Lagrangian multipliers Λ_k and maximize the function

$$Y = \operatorname{Re}\langle 0 | \phi_0 \rangle + \sum_j \Lambda_j (u_j^2 + v_j^2 - 1).$$
(4.5)

However, if the operator L_k , defined as

$$L_k = u_k \frac{\partial}{\partial v_k} - v_k \frac{\partial}{\partial u_k}, \qquad (4.6)$$

is introduced then the same result is obtained regardless of whether it is applied to X or Y.⁹

If the operator L_k is applied to Eq. (4.2) then the result must be zero

$$L_k \operatorname{Re}\langle 0 | \phi_0 \rangle = 0. \tag{4.7}$$

Substituting Eq. (4.4) into Eq. (4.7) and performing the differentiation gives

$$\operatorname{Re}\langle 0 | \alpha_k^{\dagger} \alpha_{-k}^{\dagger} | \phi_0 \rangle = 0, \qquad (4.8)$$

¹⁸ W. Brenig, Nucl. Phys. 4, 363 (1957).

which is the same as Eq. (2.6) for the PCDD. This criterion gives a great deal of insight into the meaning of a previously abstruse principle, since it is natural to choose the QP such that the unperturbed ground state is the best approximation to the true ground state. The perturbation corrections to $|\phi_0\rangle$ would then of course be smallest.

V. LEAST LABOR

For the single-particle model⁸ the criterion of "least labor for the most accuracy" was suggested in a remark by Dalgarno.¹⁹ Although this criterion is not well defined or specific, it can be used to judge the criteria which have been previously proposed. The condition that the diagram of Fig. 1 vanish identically certainly gives a simple equation that is the same as the PCDD in first order. It also corresponds to minimizing the unperturbed ground-state energy.³ Since this condition gives the simplest equation for the coefficients, it could be chosen. Then the corrections to all the other properties could be calculated from perturbation theory. However, if higher order corrections to the energy gap in Fermi systems are calculated from the QP self-energy²⁰ by perturbation theory using the first-order coefficients, Henley and Wilets' have shown that the results will not be in agreement with the self-consistent solution for the energy gap based on the PCDD because the equations are nonlinear, non-Fredholm integral equations. But it is no more work to solve the equations obtained from the PCDD at least partly in a self-consistent way than it is to use perturbation theory.

In order to illustrate this point, the equations of Henley and Wilets' will be considered. If the secondorder correction to the energy gap is calculated from the self-energy, the dressed energy gap $\tilde{\Delta}$ is²¹

$$\tilde{\Delta} = f \Delta I_1(\Delta) - f^2 \Delta I_2(\Delta), \qquad (5.1)$$

where f is the strength of the interaction, Δ is the gap obtained from setting Fig. 1 equal to zero, and the function I_1 for sufficiently small gaps is

$$I_1(\Delta) = c_1 \ln \left(b/\Delta \right), \qquad (5.2)$$

where c_1 and b are constants. For the sake of illustration, I_2 will be assumed to have the same form as I_1 , but this is not necessarily a good assumption²¹ and is not really necessary for the argument.

If the coefficients are obtained by setting Fig. 1 equal to zero, the gap Δ is given by the solution to the equation obtained from only the first-order term in Eq. (5.1)

$$\Delta = f \Delta I_1(\Delta) , \qquad (5.3)$$

which has the BCS solution

$$\Delta = b \exp\{-1/fc_1\}.$$
 (5.4)

 ¹⁹ A. Dalgarno, Rev. Mod. Phys. 35, 490 (1963).
 ²⁰ D. H. Kobe, Ann. Phys. (N. Y.) 28, 400 (1964).
 ²¹ D. H. Kobe, Quantum Chemistry Group, Uppsala, Sweden, Report No. 144, 1965 (unpublished); Ann. Phys. (N. Y.) (to be published). published).

Equation (5.4) can be substituted into Eq. (5.1) to give the gap obtained from perturbation theory⁷

$$\tilde{\Delta}_{\rm PT} = \Delta \left[1 - (fc_1)c_2/c_1^2 \right], \qquad (5.5)$$

which is the solution to the problem using the coefficients obtained from the "simplest" criterion that Fig. 1 vanish.

However, if the PCDD is used to second order to determine the coefficients, and the self-energy is also calculated to second order, then Eq. (5.1) for the energy gap becomes²²

$$\tilde{\Delta} = f \tilde{\Delta} I_1(\tilde{\Delta}) - f^2 \tilde{\Delta} I_2(\tilde{\Delta}), \qquad (5.6)$$

which is the equation to be solved self-consistently. Now the $\tilde{\Delta}$ can be *cancelled* from Eq. (5.6), which is the main part of the self-consistent calculation. Solving the resultant equation self-consistently gives

$$\tilde{\Delta}_{\rm SC} = \Delta \exp\{-c_2/c_1^2 [1 - fc_2/c_1]\}, \qquad (5.7)$$

which does not reduce to Eq. (5.5) as f goes to zero. This point was emphasized by Henley and Wilets.⁷

If the second term is much less than the first term in Eq. (5.6), i.e., if $f_{c_2}/c_1 \ll 1$, then perturbation theory can be applied to Eq. (5.6) *after* the $\tilde{\Delta}$ has been cancelled. The equation to be solved is then

$$1 = fI_1(\tilde{\Delta}) - f^2 I_2(\Delta), \qquad (5.8)$$

which has the self-consistent-perturbation-theory solution

$$\tilde{\Delta}_{\text{SCPT}} = \Delta \exp\{-(c_2/c_1^2) [1 + fc_2/c_1]\}, \quad (5.9)$$

which can be obtained from Eq. (5.7) in the case $fc_2/c_1 \ll 1$. Therefore, perturbation theory is valid after the self-consistent cancellation has taken place, which Henley and Wilets⁷ do not mention.

The point which we want to make here, however, is that there is no more labor in solving Eq. (5.8) than there is in solving Eq. (5.1) even in the case where the function I_2 is complicated and does not have the same form as I_1 . The cancellation of $\tilde{\Delta}$ is the main part of the self-consistent solution, and cannot be done in Eq. (5.1). Of course, to obtain Eq. (5.6) second-order corrections must be calculated for both the self-energy²⁰ and the PCDD, whereas, to obtain Eq. (5.1), only second-order corrections to the self-energy need be calculated. Since the form of Eq. (5.9) cannot be obtained by higher order perturbation corrections to Eq. (5.5), it is essential to use the PCDD or other criteria equivalent to it to obtain meaningful results. This is no disadvantage, however, since the criteria proposed here are compatible with the criterion of least labor.

VI. CONCLUSION

In this paper the question as to the best choice of the coefficients in the Bogoliubov canonical transformation to quasiparticles has been considered. Several different criteria have been proposed and/or analyzed to determine the "best" QP. They are:

(1) The principle of compensation of dangerous diagrams formulated by Bogoliubov,^{2,5} which removes divergences from the perturbation expansion of the ground state. For the last seven years this criterion has been the only general criterion.²³

(2) The quadratic part of the reaction operator can be diagonalized. This criterion is a generalization of the Brillouin-Brueckner condition.^{16,17}

(3) The QP vacuum state or BCS ground state can be chosen to have maximum overlap with the true ground-state vector.

(4) The criterion of "least labor for the most accuracy" is compatible with the criteria above.

It has been shown that criteria (2) and (3) are equivalent to criterion (1).

The criterion of maximum overlap of the true ground state with the BCS ground state has much more physical significance than the other criteria, since it means that the BCS ground state should be as close as possible to the true ground state. It therefore gives some real insight into the foundations of the canonical transformation method.

ACKNOWLEDGMENTS

I would like to thank Dr. V. H. Smith, Jr., for many discussions of his work on the single-particle model with Dr. Kutzelnigg. I am also very grateful to Professor P. O. Löwdin for the opportunity of coming to the Quantum Chemistry Group and his interest in my work. Professor W. B. Cheston first introduced me to the principle of compensation of dangerous diagrams, and I would like to express my gratitude to him.

 $^{^{22}}$ Henley and Wilets inadvertently leave out the gap on the right side in their Eq. (4.1) of the first part of Ref. 7.

²³ The minimization of the unperturbed ground-state energy only gives the PCDD in lowest order and is inadequate.