Perturbation Expansions and Functional Integrals in the Theory of Superconductivity*

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A functional integral representation of the partition function for a superconductor is derived by conventional perturbation-theoretic techniques. The derivation involves a generalization of the ladder diagram expansion by means of a trick due to Gaudin, and the result turns out to be a variation of the functional integral derived by Hubbard. A saddle-point approximation then leads to the usual Bardeen-Cooper-Schrieffer (BCS) equations. Although this approximation is mathematically unjustified, its predictions seem to be accurate. In particular, a very literal interpretation of the saddle-point method is supported by flux-quantization experiments.

I. INTRODUCTION

IT is fairly well known that a systematic derivation of the BCS[1] theory of superconductivity may be achieved by functional integral methods. This was first pointed out in a brief letter by Hubbard.[2] The most complete exposition is that of Mühlschlegel[3] who has used a functional integral technique to prove that the BCS solution for the truncated pair model is asymptotically exact in the limit of large volume. Although the functional integral method has not yet yielded results of practical importance, it does have a certain formal attraction. In particular, the method provides a representation of the partition function which may be continued analytically through the phase transition. In fact, a zeroth-order approximation to the integral, which turns out to be exact for the pair model, is a realization of Landau's phenomenological theory of second-order phase transitions.[4]

Such a result is obviously beyond the reach of conventional perturbation expansions. Even with the Green's function[5] methods one necessarily obtains, say, the free energy in terms of two completely different analytic functions—one valid only above, and the other only below, the transition temperature. Nevertheless, it is possible to use the conventional rules of perturbation theory in an unorthodox way and arrive at an expression for the partition function in the form of a functional integral. This is the main point of the present paper.

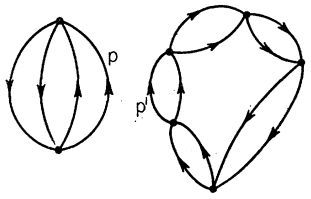

FIG. 1. A contribution to the partition function composed of closed ladder diagrams.

The functional integral so derived is equivalent to that obtained by more direct means by Hubbard and Mühlschlegel. We shall be able to see this relationship clearly, although we shall not attempt a rigorous demonstration of equivalence. What is important is that the functional integral here has an unambiguous perturbation-theoretic interpretation; and the establishment of this connection adds to the understanding of both methods.

At this point some comments concerning the structure of the perturbation expansion are in order. Consider as an example Thouless' calculation of the free energy of a Fermi gas with weak attractive interactions.[6] Thouless sums the so-called "ladder diagrams," typical examples of which are shown in Fig. 1. He finds that, at exactly the BCS critical temperature, bound-pair states become energetically favorable and the free energy develops a branch point. There is no sensible way of continuing analytically around this singularity in the complex temperature plane. In fact, we know that such a singularity never can occur in the correct free energy for any finite, positive temperature.

In some intuitive sense, it is obvious what has gone wrong. Thouless has used the linked-cluster theorem and has summed only a small class of perturbation diagrams; thus his result violates the Pauli principle. For example, the contribution from the term $\mathbf{p}=\mathbf{p}'$ in Fig. 1 should, in principle, be cancelled by the diagram in Fig. 2 in which the two lines have been exchanged. But this second diagram has been omitted in Thouless' calculation. Roughly speaking, the singularity in the energy occurs because each electron has been bound into a pair infinitely many times. In order to avoid this divergence one presumably must include all the ex-

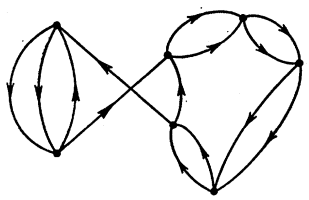

FIG. 2. An exchange correction to Fig. 1.

* Supported by the National Science Foundation.
[1] J. Bardeen, L. Cooper, J. R. Schrieffer, Phys. Rev. **108**, 1175 (1957).
[2] J. Hubbard, Phys. Rev. Letters **3**, 77 (1959).
[3] B. Mühlschlegel, J. Math. Phys. **3**, 522 (1962).
[4] L. D. Landau and E. M. Lifshitz, *Statistical Physics* (Addison-Wesley Publishing Company Inc., Reading, Massachusetts, 1958), p. 434.
[5] L. P. Gor'kov, Zh. Eksperim. i Teor. Fiz. **34**, 735 (1958) [English transl.: Soviet Phys.—JETP **7**, 505 (1958)].
[6] D. J. Thouless, Ann. Phys. (N. Y.) **10**, 553 (1960).

change corrections to the ladder diagrams. But we can generate every term in the perturbation expansion by exchanging lines within and between unlinked ladder diagrams. Thus, it seems that if we want to examine the phase transition, we must take into account all possible diagrams. The inevitable approximations must not be based on any truncation of the perturbation expansion.

The reformulation of perturbation theory to be discussed here has its origins in a remarkable paper by M. Gaudin.[7] After a considerable amount of combinatorial work (bearing no obvious resemblance to that to be presented here), Gaudin is able to sum a simple contribution from every diagram and arrive at an approximate expression for the partition function which is sensible on both sides of a transition temperature. In the limit of infinite volume, this expression yields exactly the correct transition temperature and free energy for the BCS pair model with a separable interaction. Later on in this paper we shall see why Gaudin's method turns out to be exact.

The crucial features of Gaudin's work to be adopted here are the following. We shall use his diagrammatic notation, which is very convenient for the study of pairing effects. More important fundamentally, we shall expand the partition function directly rather than use the linked-cluster theorem. Combinatorial problems turn out to be easier when we can relax the condition that all diagrams must be connected. Furthermore, the partition function apparently is an analytic function of the interaction strength throughout a large region including the transition, whereas the linked cluster expansion for the free energy has a radius of convergence about the transition point which goes to zero in the limit of infinite volume. Thus, by working directly with the partition function we are on firmer ground mathematically. In any case, we shall be careful to keep the volume of the system large but finite in order to be able to make analytic continuations through the transition. For a discussion of the analytic properties of Gaudin's partition function, the reader should consult a recent note by the author in collaboration with Balian.[8]

The scheme of this paper is as follows. The perturbation-theoretic derivation of the functional integral is contained in Sec. II. Sections III and IV are then devoted to the evaluation of this integral. We shall see that the BCS results are obtained from a zeroth-order saddle-point approximation—the approximation which corresponds to Landau's phenomenological theory of second-order phase transitions. Although this method is very unsound mathematically, it leads to remarkably good results for the superconductor. We shall emphasize this fact in Sec. V by pointing out that a very literal interpretation of the saddle-point method is supported by the flux-quantization experiments. Finally, an Appendix contains a generalization of the results of Sec. II to more complicated two-body interactions.

II. DERIVATION OF THE FUNCTIONAL INTEGRAL

We consider the system defined by the Hamiltonian

$$H-\mu N=\sum_{\mathbf{p},\sigma}\epsilon_{\mathbf{p}}a_{\mathbf{p},\sigma}{}^{\dagger}a_{\mathbf{p},\sigma}$$

$$-\frac{g}{2\Omega}\sum_{\mathbf{p},\mathbf{p}',\mathbf{Q},\sigma}a_{\mathbf{p}+\mathbf{Q},\sigma}{}^{\dagger}a_{-\mathbf{p},-\sigma}{}^{\dagger}a_{-\mathbf{p}',-\sigma}a_{\mathbf{p}'+\mathbf{Q},\sigma}. \quad (2.1)$$

Here $a_{\mathbf{p},\sigma}$ and $a_{\mathbf{p},\sigma}{}^{\dagger}$ are the annihilation and creation operators for Fermions of momentum $\mathbf{p}$, spin σ. The kinetic energies $\epsilon_{\mathbf{p}}$ are measured from the chemical potential μ. Ω is the quantization volume relevant to periodic boundary conditions. The potential energy consists of a simple separable interaction between electrons of opposite spin but not necessarily opposite momentum. The restriction to opposite spins just eliminates inconsequential complications in the following work. The separability of the potential, however, plays an important role. In an Appendix to this paper it is shown that these methods can be generalized to deal with a more realistic form of the two-body interaction. In order to describe the separable interaction by a single coupling constant g, we shall have to understand that all sums over $\mathbf{p}$ are restricted to a band containing a finite number of states per unit volume. Note that we have written (2.1) so that positive g implies an attractive interaction. We shall be interested in this case only.

The perturbation expansion to be used is that of Bloch and De Dominicis[9] in the propagator version formulated by Luttinger and Ward.[10] Let Z denote the grand partition function

$$Z=\mathrm{Tr}\,\exp\{-\beta(H-\mu N)\}, \quad (2.2)$$

where β is the inverse temperature; and let Z_0 denote the value of Z for no interactions ($g=0$). Then Z/Z_0 is the sum of the contributions associated with all topologically distinct vacuum to vacuum diagrams.

The basis for all of the following combinatorial development is the unusual diagrammatic notation which was introduced by Gaudin.[7] We shall draw the four-Fermion interaction vertices as shown in Fig. 3. A typical diagram occurring in the expansion of Z/Z_0 then consists of a number of "stars" whose points are

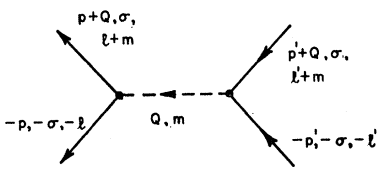

FIG. 3. Diagrammatic representation of the basic interaction.

[7] M. Gaudin, Nucl. Phys. **20**, 513 (1960).
[8] R. Balian and J. S. Langer, Phys. Rev. **132**, 958 (1963).
[9] C. Bloch and C. T. De Dominicis, Nucl. Phys. **7**, 459 (1958); **10**, 181 (1958).
[10] J. M. Luttinger and J. C. Ward, Phys. Rev. **118**, 1417 (1960).

connected in various ways by the dashed "interaction" lines. One such diagram is shown in Fig. 4.

The rules for evaluating these diagrams are:

1. For each electron line write a factor

$$\beta^{-1}[\epsilon_{\mathbf{p}}-(i\pi l/\beta)]^{-1},$$

where l is an odd integer. Momentum $\mathbf{p}$ and "energy" l must be conserved in each interaction. The simplest way to keep the momentum and energy variables straight is to associate with each interaction line the proper values of $\mathbf{Q}$ and m (even integer) as indicated in Fig. 3. It should be emphasized that $\mathbf{Q}$ and m do not correspond to momentum and energy transfers in the usual sense but rather must be understood as the total momentum and energy of the pair of electrons which is in interaction.

2. For each interaction line write a factor $g\beta/\Omega$.

3. For each star write a factor $\frac{1}{2}$ to correct for overcounting in the spin sum.

4. Write factors (-1) for each star and each interaction line.

5. Sum over all $\mathbf{p}$, σ, l, etc.

All of these rules should be familiar except for the determination of the sign. The usual prescription calls for a factor (-1) for each closed Fermion loop. [Remember we have written the interaction in (2.1) with $-g$.] A star, however, is *not* a closed loop. In order to trace the usual closed-loop pictures corresponding to a star diagram, we must follow alternate electron and interaction lines from star to star. The structure is rather complicated; but it is easy to convince oneself that if we exchange the destination points of any two interaction lines, we always open or close an even number of loops, and thus do not change the explicit sign. (This would not be true if we allowed parallel spin interactions.) It follows that we can determine the sign of any diagram in which all the interaction lines have been inserted as shown in Fig. 5. The same diagram in standard notation is shown in Fig. 6. It is obvious that the number of closed loops, thus the number of explicit minus signs, equals the number of interactions plus the number of stars.

We turn now to the classification of the diagrams. The orthodox linked-cluster expansion would require that we sort the diagrams according to how the constituent stars are connected by the interaction lines. As we have seen, however, the technique of isolating unlinked parts of a diagram leads, in practice, to violations of the Pauli principle. Therefore, we shall take just the opposite point of view; that is, we shall classify diagrams according to the particular stars which they contain and then sum over all ways of connecting these stars by the interaction lines.

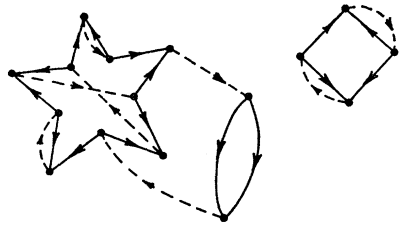

FIG. 4. A typical star diagram.

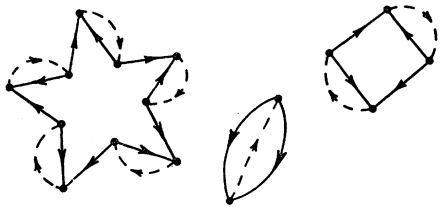

FIG. 5. A rearrangement of the interaction lines in Fig. 4. The over-all sign of the diagram is preserved.

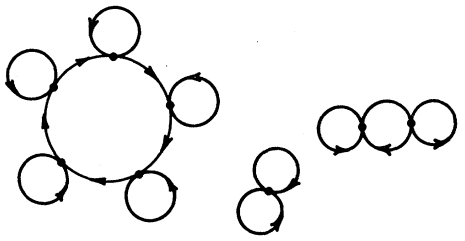

FIG. 6. Conventional diagrammatic notation for Fig. 5.

The above program requires a description of the diagrams which is somewhat more detailed than usual. To be precise, we must at first treat interactions with different m, $\mathbf{Q}$ values as if they were essentially different from one another. For simplicity, let us use the symbol α to denote the four-vector $(m,\mathbf{Q})$. A given diagram then consists of a number of stars connected in a certain way by, say, n_α interaction lines α, $n_{\alpha'}$ lines α', etc. The sums over the α's will be performed at a later stage of the calculation than the sums over those momenta and energies associated with the electron lines within the stars.

Any given star contains a certain number of external vertices from which interaction lines α emerge. The number of such vertices will be denoted by the symbol $N_{\mathcal{S}}(\alpha)$, $\mathcal{S}$ denoting the particular star under consideration. Similarly, there will be $M_{\mathcal{S}}(\alpha)$ internal vertices where interaction lines α enter the star. A complete description of the star thus consists of the set of numbers $N_{\mathcal{S}}(\alpha)$, $N_{\mathcal{S}}(\alpha')$, $\cdots$, $M_{\mathcal{S}}(\alpha)$, $\cdots$, along with an indication of the order in which the various vertices occur. By virtue of the way in which the star is constructed, we have automatically:

$$\sum_\alpha N_{\mathcal{S}}(\alpha)=\sum_\alpha M_{\mathcal{S}}(\alpha) \tag{2.3}$$

and

$$\sum_\alpha N_{\mathcal{S}}(\alpha)\alpha=\sum_\alpha M_{\mathcal{S}}(\alpha)\alpha. \tag{2.4}$$

These equations state simply that the number of internal vertices equals the number of external vertices

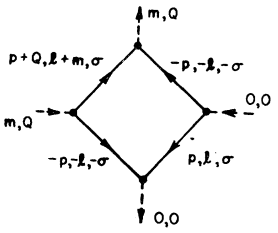

FIG. 7. The sample star whose numerical value is given in Eq. (2.5).

and that energy and momentum are conserved at each vertex.

Next let us denote by $-\Omega K_{\mathcal{S}}$ the numerical contribution of the star $\mathcal{S}$. To be precise, $K_{\mathcal{S}}$ contains the propagator factors of rule 1, factors $-g\beta/\Omega$ for each external vertex according to rules 2 and 4, and the factor $\frac{1}{2}$ of rule 3. $K_{\mathcal{S}}$ also contains a sum over the $\mathbf{p}$, σ, l which run around the star. For example, for the star shown in Fig. 7 we have

$$-\Omega K_{\mathcal{S}}=-\frac{1}{2}\left(-\frac{g\beta}{\Omega}\right)^2\frac{1}{\beta^4}$$

$$\times\sum_{\mathbf{p},l,\sigma}1\Big/\left[\epsilon_{\mathbf{p}}-\frac{i\pi l}{\beta}\right]\left[\epsilon_{\mathbf{p}}+\frac{i\pi l}{\beta}\right]^2\left[\epsilon_{\mathbf{p}+\mathbf{Q}}-\frac{i\pi}{\beta}(l+m)\right];$$

$$N_{\mathcal{S}}(\mathbf{Q},m)=M_{\mathcal{S}}(\mathbf{Q},m)=N_{\mathcal{S}}(0,0)=M_{\mathcal{S}}(0,0)=1. \quad (2.5)$$

Consider now a complete diagram Γ consisting of a number of stars connected in a particular way by a corresponding number of interaction lines with fixed values of α. Suppose that each star $\mathcal{S}$ appears ν_s times in Γ. Then the contribution of Γ to the partition function is

$$(Z/Z_0)_\Gamma=\prod_{\mathcal{S}}(-\Omega K_{\mathcal{S}})^{\nu_s}. \quad (2.6)$$

There are several restrictions on the way in which these diagrams can be formed. The number of α interaction lines must equal the total number of external α vertices which, in turn, must equal the total number of internal α vertices. It is convenient to write these restrictions as follows:

$$n_\alpha=\tfrac{1}{2}\sum_{\mathcal{S}}\nu_s[N_{\mathcal{S}}(\alpha)+M_{\mathcal{S}}(\alpha)]; \quad (2.7)$$

and

$$\sum_{\mathcal{S}}\nu_s N_{\mathcal{S}}(\alpha)=\sum_{\mathcal{S}}\nu_s M_{\mathcal{S}}(\alpha). \quad (2.8)$$

Note that, unlike Eqs. (2.3) and (2.4), these restrictions are not automatically satisfied by any product of the form (2.6) which we might care to write.

Given the diagram Γ, there exist a number of other diagrams which may be obtained simply by rearranging the interaction lines, all of which diagrams have the same numerical value. There are, in fact,

$$\prod_\alpha n_\alpha! \quad (2.9)$$

ways of rearranging the interaction lines; but many of these arrangements lead to diagrams which are topologically identical. To correct for this, we must divide (2.9) by the number of ways we can rearrange the stars so as to leave the diagram invariant. There are

$$\prod_{\mathcal{S}}\nu_s! \quad (2.10)$$

ways of exchanging identical stars among themselves. Furthermore, individual stars may have rotational symmetries. Let $W_{\mathcal{S}}$ be the number of rotations which leave the star $\mathcal{S}$ invariant. Then the entire diagram is invariant under

$$\prod_{\mathcal{S}}(W_{\mathcal{S}})^{\nu_s} \quad (2.11)$$

such rotations. If we divide (2.9) by (2.10) and (2.11), we may write the complete partition function in the form

$$Z/Z_0=\sum_{\{\nu\}}\prod_\alpha n_\alpha!\prod_{\mathcal{S}}\frac{1}{\nu_s!}\left(-\frac{\Omega}{W_{\mathcal{S}}}K_{\mathcal{S}}\right)^{\nu_s}, \quad (2.12)$$

where the sum over $\{\nu\}$ represents the sum over all sets of integers ν_s which satisfy the relations (2.7) and (2.8).

The final step in this derivation is to rewrite Eq. (2.12) in such a form that the restrictions (2.7) and (2.8) are satisfied automatically. We then shall be left with an expression involving only a sum over independent stars. We use the integral representation for the gamma function in the form

$$n_\alpha!=\Omega\int_0^\infty dt_\alpha(\Omega t_\alpha)^{n_\alpha}e^{-\Omega t_\alpha}. \quad (2.13)$$

If we insert (2.13) into (2.12) with

$$(\Omega t_\alpha)^{n_\alpha}=(\Omega t_\alpha)^{\frac{1}{2}\sum_s\nu_s[N_s(\alpha)+M_s(\alpha)]}, \quad (2.14)$$

then we have satisfied Eq. (2.7). Note that Eq. (2.14) implies simply that we insert a factor $(\Omega t_\alpha)^{1/2}$ at each α vertex (external or internal) on each star in the diagram.

In a similar spirit we may account for (2.8) by inserting into (2.12) the integral representation for the Kronecker delta symbol:

$$\delta_{\sum_s\nu_s N_s(\alpha),\sum_s\nu_s M_s(\alpha)}$$

$$=\frac{1}{2\pi}\int_0^{2\pi}d\phi_\alpha\exp\{i\phi_\alpha\sum_{\mathcal{S}}\nu_s[N_{\mathcal{S}}(\alpha)-M_{\mathcal{S}}(\alpha)]\}. \quad (2.15)$$

This insertion is equivalent to writing a factor $\exp(i\phi_\alpha)$ at each external α vertex and a factor $\exp(-i\phi_\alpha)$ at each internal α vertex.

We can summarize the last few steps as follows. For any given star $\mathcal{S}$ (described by the set of numbers $N_{\mathcal{S}}(\alpha)$, $N_{\mathcal{S}}(\alpha')$, $\cdots$, $M_{\mathcal{S}}(\alpha)$, $M_{\mathcal{S}}(\alpha')$, $\cdots$, and the order in which the vertices occur) we must compute a function

$-\Omega K_{\mathcal{S}}\{t,\phi\}$. Here the symbol $\{t,\phi\}$ represents the complete set of integration variables t_α, $t_{\alpha'}$, $\cdots$, and ϕ_α, $\phi_{\alpha'}$, $\cdots$. In addition to the propagator factors of rule 1 and the factor $\frac{1}{2}$ of rule 3, the new $K_{\mathcal{S}}$ contains a factor $(-g\beta t_\alpha)^{1/2}\exp(i\phi_\alpha)$ for each external α vertex and a factor $(-g\beta t_\alpha)^{1/2}\exp(-i\phi_\alpha)$ for each internal α vertex. In terms of this function the partition function is:

$$Z/Z_0=\sum_{\{\nu\}}\prod_\alpha\left[\frac{\Omega}{2\pi}\int_0^\infty e^{-\Omega t_\alpha}dt_\alpha\int_0^{2\pi}d\phi_\alpha\right]\times\prod_{\mathcal{S}}\frac{1}{\nu_{\mathcal{S}}!}\left[-\frac{\Omega}{W_{\mathcal{S}}}K_{\mathcal{S}}\{t,\phi\}\right]^{\nu_{\mathcal{S}}}. \quad (2.16)$$

Because the sum over $\{\nu\}$ is now unrestricted, we have

$$Z/Z_0=\prod_\alpha\left[\frac{\Omega}{2\pi}\int_0^\infty dt_\alpha\int_0^{2\pi}d\phi_\alpha\right]e^{-\Omega Y\{t,\phi\}}, \quad (2.17)$$

where

$$Y\{t,\phi\}\equiv\sum_\alpha t_\alpha+\sum_{\mathcal{S}}\frac{1}{W_{\mathcal{S}}}K_{\mathcal{S}}\{t,\phi\}. \quad (2.18)$$

This is the desired representation of the partition function.

The connection between (2.17) and the more conventional functional integral forms may be established by making the transformation

$$(t_\alpha)^{1/2}e^{i\phi_\alpha}=x_{\alpha,1}+ix_{\alpha,2}. \quad (2.19)$$

Then we have

$$Z=\prod_{\substack{\alpha\\ i=1,2}}\left(\frac{\Omega^{1/2}}{\pi}\int_{-\infty}^\infty dx_{\alpha,i}\right)\exp[-\Omega\sum_{\alpha,i}x_{\alpha,i}^2]\,\vartheta\{x\}, \quad (2.20)$$

where

$$\vartheta\{x\}\equiv Z_0\exp\left[-\Omega\sum_{\mathcal{S}}\frac{1}{W_{\mathcal{S}}}K_{\mathcal{S}}\{x\}\right]. \quad (2.21)$$

The $x_{\alpha,i}$'s now may be interpreted as a set of random variables with Gaussian distribution which play the role of Fourier coefficients in a pairing potential.

$$\left(\frac{g}{\beta}\right)^{1/2}\sum_{\mathbf{p},\mathbf{Q},m}(x_{m,\mathbf{Q},1}+ix_{m,\mathbf{Q},2})\times\exp\left(\frac{2\pi im\tau}{\beta}\right)a_{\mathbf{p}+\mathbf{Q},\sigma}{}^\dagger a_{-\mathbf{p},-\sigma}{}^\dagger+\text{h.c.} \quad (2.22)$$

It should be apparent that a perturbation expansion in powers of this time-dependent potential generates the star diagrams which define ϑ. The "time" variable τ $(0<\tau<\beta)$ really is to be interpreted as the Feynman ordering parameter[11] as used by Hubbard[2] and Mühlschlegel.[3] For our purposes, the τ dependence appears in (2.22) simply to introduce the proper energy (m) dependence at the vertices where pairs are created and annihilated. The final result is that $\vartheta\{x\}$ is a sort of partition function for independent particles moving in a random pairing potential; that is, $\vartheta\{x\}$ is a functional of the potential. The exact partition function Z is then given by (2.20) as the Gaussian average of $\vartheta\{x\}$, which is a functional integral.

[11] R. Feynman, Phys. Rev. 84, 108 (1951).

III. GENERAL FEATURES OF THE INTEGRAL

We turn our attention now to the problem of evaluating (2.17). In particular, we shall want to compute the grand canonical potential.

$$\Psi=\lim_{\Omega\to\infty}\left\{-\frac{1}{\beta\Omega}\ln Z\right\}. \quad (3.1)$$

Note that the function Y has been constructed in such a way that the only explicit volume dependence enters through the sum over $\mathbf{p}$. The functions of $\mathbf{p}$ which are summed over are all well behaved, and we may replace this sum by an integral.

$$\frac{1}{\Omega}\sum_{\mathbf{p}}\to\frac{1}{(2\pi)^3}\int d^3p.$$

With this replacement, Y becomes completely independent of Ω. This is very important because it seems to imply that Y is a slowly varying function of its arguments; that is, it apparently has no volume-dependent structure or oscillations whose frequencies increase with the size of the system.

It now becomes very tempting to evaluate (2.17) by a saddle-point method. Presumably we need only look for the minimum of the real part of the slowly varying function Y. At this point the integrand in (2.17) will have a peak which, in the limit of very large Ω, should dominate the partition function. Such a procedure seems even more attractive when one considers its physical significance. A point in x space determines a particular pairing potential (2.22). A situation in which the partition function is accurately determined by the value of Y very near just one such point, say $\{\bar{x}\}$, clearly is a case in which the self-consistent field method is good. We therefore expect ReY to be minimized at an $\{\bar{x}\}$ such that (2.22) is the BCS self-consistent pairing potential. As we shall see, this is indeed what happens. Furthermore, this procedure is in close analogy with Landau's phenomenological theory of second-order phase transitions.[4] Y plays the role of Landau's free-energy function, here a function of a large set of order parameters $\{x\}$. In the disordered phase presumably $\{\bar{x}\}$ lies at the origin and the pairing potential vanishes. As we pass through the transition temperature, $\{\bar{x}\}$ moves away from the origin and we obtain the ordered phase.

All of the above arguments would be exactly correct if the set $\{x\}$ consisted of only a finite number of

variables. But we must have a different variable x for every allowed $m, \mathbf{Q}$; and the number of allowed $\mathbf{Q}$'s becomes infinite as the volume Ω goes to infinity. This is what makes (2.17) a nontrivial functional integral.

To see the sort of difficulties which arise when the dimensionality of x space becomes infinite, consider the integral

$$\Xi_G \equiv \prod_{\alpha=1}^{G} \left(\frac{\Omega^{1/2}}{\pi} \int_{-\infty}^{\infty} dx_\alpha \right) \exp[\Omega(a - \sum_\alpha b_\alpha^2 x_\alpha^2)], \quad (3.2)$$

which is essentially the form of the integral we shall obtain when we expand $\ln \vartheta\{x\}$ in (2.20) up to terms quadratic in the x_α's. Ξ_G is easily evaluated to give

$$\Xi_G = e^{\Omega a} \prod_{\alpha=1}^{G} \left(\frac{1}{b_\alpha} \right); \quad (3.3)$$

$$\frac{1}{\Omega} \ln \Xi_G = a - \frac{1}{\Omega} \sum_{\alpha=1}^{G} \ln b_\alpha. \quad (3.4)$$

If G is a finite constant independent of Ω, then only the first term a remains in (3.4) in the limit $\Omega \to \infty$. This is characteristic of a conventional saddle-point integral, and we may expect higher terms in the expansion of $\ln \vartheta$ to generate an expansion of $\ln \Xi_G$ in powers of Ω^{-1}. But if G is proportional to Ω, then both terms on the right-hand side of (3.4) remain of order unity, and the saddle-point method is not necessarily an expansion in powers of anything very sensible. In fact it may be quite impossible to generate any systematic sequence of higher approximations in this way.

Note that, in evaluating (3.2), we obtain appreciable contributions to the integral from points in x space where all of the x_α's are of order $\Omega^{-1/2}$. At such a point the quantity

$$\sum_\alpha b_\alpha^2 x_\alpha^2$$

is of order G/Ω, which remains finite according to our assumptions. In other words, in order for (3.2) to be a good approximation to an integral like (2.20), the quadratic approximation to $\ln \vartheta\{x\}$ must be accurate everywhere within a G-dimensional ellipse whose typical radius is of order unity. It is certainly not obvious that this is the case for (2.20). For example, the pairing potential (2.22) is a linear combination of G terms each of order $\Omega^{-1/2}$, which clearly doesn't fulfill our hopes of a smooth, volume-independent function $Y\{x\}$.

At this point it should be clear, however, that the BCS truncated pair model does fit very nicely into the formalism we have outlined. This model is obtained from the Hamiltonian (2.1) by restricting the interaction to only those pairs for which the total momentum $\mathbf{Q}$ is zero. The subscript α now reduces to m, which ranges over the even integers. If the sum over $\alpha = m$ in (3.4) converges uniformly (which it does if we are sufficiently careful), we may take G equal to some large integer M and take the limit $M \to \infty$ after we take $\Omega \to \infty$. Thus G is effectively finite and the saddle-point method generates an expansion in powers of Ω^{-1}. The leading term in this expansion is the BCS solution, which therefore is asymptotically exact in the limit of large volume.

But from this point of view the BCS model is highly unrealistic because the interaction is effectively volume-dependent. The BCS theory is analogous to the molecular-field solution for the Ising model which is obtained as an exact result by letting the range of the interaction go to infinity before taking the limit of infinite volume. A much more satisfactory treatment of the superconductor might be one in which the interaction has the form

$$\frac{g}{2\Omega} \sum_{\mathbf{p},\mathbf{p}',\mathbf{Q},\sigma} \Delta(\mathbf{Q}) a_{\mathbf{p}+\mathbf{Q},\sigma}^\dagger a_{-\mathbf{p},-\sigma}^\dagger a_{-\mathbf{p}',-\sigma} a_{\mathbf{p}'+\mathbf{Q},\sigma}, \quad (3.5)$$

and the limit

$$\Delta(\mathbf{Q}) \to \delta(\mathbf{Q})$$

is taken *after* $\Omega \to \infty$. An analysis of this sort has been performed for the one-dimensional Ising model by Baker.[12] No such rigorous solution has yet been demonstrated for the superconductor. It is likely, but by no means obvious, that the BCS solution would be recovered in this way. It is even more likely that the problem is not soluble as stated.

IV. SADDLE-POINT APPROXIMATION

We proceed now to an evaluation of Ψ by means of the saddle-point method, with the understanding that the technique is at best an unjustified approximation.

A. The Normal Phase

The accepted criterion for "normality" of a many-Fermion system is that all thermodynamic functions be well described by a perturbation expansion in powers of the interaction strength. If the system described by (2.17) is to be normal, the minimum value of $\mathrm{Re}Y$ within the region of integration must occur at the origin in t space. To see this, note simply that the interaction strength g always occurs in Y in the combination gt_α. Thus, for any fixed values of the t's, the expansion of Y in powers of the t's is also an expansion in g.

The first term in this expansion may be computed

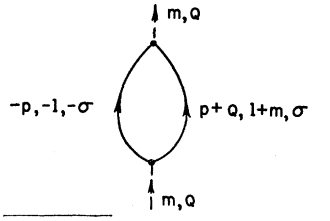

FIG. 8. Diagrammatic representation of λ_α. The numerical value is given in Eq. (4.1).

[12] G. A. Baker, Phys. Rev. **122**, 1477 (1961).

quite easily. The only star which contributes a term just proportional to t_α is the simple one shown in Fig. 8. Its contribution to Y is

$$-\frac{gt_\alpha}{2\beta\Omega}\sum_{\mathbf{p},l,\sigma}1\Big/\left[\epsilon_{\mathbf{p}}+\frac{i\pi l}{\beta}\right]\left[\epsilon_{\mathbf{p}+\mathbf{Q}}-\frac{i\pi}{\beta}(l+m)\right]$$
$$\equiv -gt_\alpha\lambda_\alpha. \quad (4.1)$$

Note that the phase angles ϕ_α cancel out. Then

$$Y\{t,\phi\}\cong\sum_\alpha t_\alpha - g\sum_\alpha t_\alpha\lambda_\alpha+O(g^2t^2). \quad (4.2)$$

The condition for ReY to be a minimum at the origin is

$$\mathrm{Re}(1-g\lambda_\alpha)>0 \quad (4.3)$$

for all α. As the temperature decreases, (4.3) will be violated first by the $\alpha=(0,0)$ term; thus the critical temperature is determined by

$$g\lambda_{0,0}=\frac{g}{2\beta_c\Omega}\sum_{\mathbf{p},l,\sigma}1\Big/\left(\epsilon_{\mathbf{p}}^2+\frac{\pi^2l^2}{\beta_c^2}\right)$$
$$=\frac{g}{2\Omega}\sum_{\mathbf{p}}\frac{1}{\epsilon_{\mathbf{p}}}\tanh\frac{\beta_c\epsilon_{\mathbf{p}}}{2}=1. \quad (4.4)$$

This is exactly the BCS equation for the transition point.

When (4.3) is satisfied, we may use (4.2) to evaluate the partition function.

$$Z/Z_0\cong\prod_\alpha\left(\Omega\int_0^\infty dt_\alpha\right)\exp\{-\Omega\sum_\alpha t_\alpha(1-\lambda_\alpha)\}$$
$$=\prod_\alpha(1-g\lambda_\alpha)^{-1}; \quad (4.5)$$

and

$$\Psi=\Psi_0+\frac{1}{\beta\Omega}\sum_\alpha\ln(1-g\lambda_\alpha), \quad (4.6)$$

where

$$\Psi_0\equiv-\frac{1}{\beta\Omega}\ln Z_0.$$

In (4.6) the sum over α converges to a quantity of order Ω, at least after we correct for misusing the propagator formalism for the lowest order diagram ($\sim g$). We recognize (4.6) as precisely Thouless' result for the sum of the ladder diagrams shown in Fig. 1.

B. The Superconducting Phase

When condition (4.3) is not satisfied, the origin in t space no longer locates a minimum of ReY within the region of integration. As suggested by the discussion in Sec. III, we now may expect to find a minimum of ReY by moving out along the axis $\alpha=(0,0)$ which corresponds to a spatially uniform pairing potential. The next step, therefore, is to evaluate Y at all points along this axis and locate a minimum. In doing this we shall recover Gaudin's results. The equation determining this minimum is the BCS gap equation; and the value of Y at this point is the correct grand canonical potential as given by Bogolyulov, Zubarev, and Tserkovnikov.[13] In addition, we shall show that this point on the $\alpha=(0,0)$ axis locates a true minimum of ReY considered as a function of all of its variables, thus justifying completion of the saddle-point approximation.

Let us denote the variable t_α for $\alpha=(0,0)$ by t_0, and the value of $Y\{t,\phi\}$ along this axis by $Y(t_0)$. If we set all the t_α's equal to zero except t_0, then $Y(t_0)$ is determined by a very simple class of stars, i.e., those in which only $\alpha=(0,0)$ interaction lines enter or emerge. The numerical value K for such a star is determined only by the number of external (or internal) vertices, say, k. According to the rules of Sec. II,

$$K_k=\frac{1}{2\Omega}\sum_{\mathbf{p},l,\sigma}\left(-\frac{gt_0}{\beta}\frac{1}{\epsilon_{\mathbf{p}}^2+(\pi^2l^2/\beta^2)}\right)^k. \quad (4.7)$$

Again, the phase angles have cancelled out. This class of stars has the highest possible rotational symmetry; a k-pointed star has k equivalent orientations, which implies that

$$W_k=k. \quad (4.8)$$

Thus, from (2.18), we have

$$Y(t_0)=t_0+\sum_k\frac{1}{2\Omega k}\sum_{\mathbf{p},l,\sigma}\left(-\frac{gt_0}{\beta}\frac{1}{\epsilon_{\mathbf{p}}^2+(\pi^2l^2/\beta^2)}\right)^k$$
$$=t_0-\frac{1}{2\Omega}\sum_{\mathbf{p},l,\sigma}\ln\left(1+\frac{gt_0}{\beta}\frac{1}{\epsilon_{\mathbf{p}}^2+(\pi^2l^2/\beta^2)}\right)$$
$$=t_0-\frac{2}{\Omega}\sum_{\mathbf{p}}\ln\left(\frac{\cosh[(\beta/2)(\epsilon_{\mathbf{p}}^2+gt_0/\beta)^{1/2}]}{\cosh\frac{1}{2}\beta\epsilon_{\mathbf{p}}}\right). \quad (4.9)$$

The minimum value of $Y(t_0)$ occurs at $t_0=s$ such that

$$\left.\frac{\partial Y}{\partial t_0}\right|_{t_0=s}=0=1-\frac{g}{2\Omega\beta}\sum_{\mathbf{p},l,\sigma}1\Big/\left(\epsilon_{\mathbf{p}}^2+\frac{\pi^2l^2}{\beta^2}+\frac{gs}{\beta}\right)$$
$$=1-\frac{g}{2\Omega}\sum_{\mathbf{p}}\frac{\tanh\frac{1}{2}\beta(\epsilon_{\mathbf{p}}^2+gs/\beta)^{1/2}}{(\epsilon_{\mathbf{p}}^2+gs/\beta)^{1/2}}. \quad (4.10)$$

That s is a minimum and, in fact, the only minimum of $Y(t_0)$ may be verified easily by inspection. Equation (4.10) is exactly the BCS equation for the gap Δ if we identify

$$\frac{gs}{\beta}\equiv\Delta^2. \quad (4.11)$$

In order to show that s locates a minimum of the

[13] N. N. Bogolyubov, D. N. Zubarev, and Yu. A. Tserkovnikov, Dokl. Acad. Nauk SSSR **117**, 788 (1958) [English transl.: Soviet Phys.—Dokl. **2**, 535 (1958)]; Zh. Eksperim. i Teor. Fiz. **39**, 120 (1960) [English transl.: Soviet Phys.—JETP **12**, 88 (1961)].

complete function Y we must consider the first terms in the Taylor series expansion about this point. These terms will be given by the class of stars whose numerical values are linear in the t_α's, $\alpha \neq (0,0)$, i.e., those stars which have any number of $\alpha=(0,0)$ vertices plus exactly two vertices for which $\alpha \neq (0,0)$. [Because of "energy" and momentum conservation, no star can have only one $\alpha \neq (0,0)$ vertex. See Eq. (2.4).] The relevant stars are illustrated in Fig. 9. For ease in interpreting these diagrams, $\alpha=(0,0)$ vertices have been marked by circles and $\alpha \neq (0,0)$ vertices by black dots. The momentum values have been omitted.

The numerical value of the sum of all stars of the form of Fig. 9(a) may be obtained by summing over all possible numbers of $\alpha=(0,0)$ vertices which may be inserted between the two $\alpha \neq (0,0)$ vertices. The result is

$$-\frac{1}{2\Omega}\sum_{\mathbf{p},l,\sigma}\frac{gt_\alpha/\beta}{\left[\epsilon_{\mathbf{p}}+\frac{i\pi l}{\beta}\right]\left[\epsilon_{\mathbf{p}+\mathbf{Q}}-\frac{i\pi(l+m)}{\beta}\right]}\frac{1}{\left[1+\frac{gt_0/\beta}{\epsilon_{\mathbf{p}}^2+(\pi^2l^2/\beta_2)}\right]}\frac{1}{\left[1+\frac{gt_0/\beta}{\epsilon_{\mathbf{p}+\mathbf{Q}}^2+[\pi^2(l+m)^2/\beta^2]}\right]}$$

$$=-\frac{gt_\alpha}{2\Omega\beta}\sum_{\mathbf{p},l,\sigma}\frac{[\epsilon_{\mathbf{p}}-(i\pi l/\beta)][\epsilon_{\mathbf{p}+\mathbf{Q}}+(i\pi(l+m)/\beta)]}{[\epsilon_{\mathbf{p}}^2+(\pi^2l^2/\beta^2)+(gt_0/\beta)][\epsilon_{\mathbf{p}+\mathbf{Q}}^2+(\pi^2(l+m)^2/\beta^2)+(gt_0/\beta)]}\equiv -t_\alpha\gamma_\alpha(t_0). \quad (4.12)$$

In a similar fashion, the numerical value of the sum of all diagrams of the form of Fig. 9(b) is

$$\frac{g^2t_0(t_\alpha t_{-\alpha})^{1/2}}{2\beta^2\Omega}\exp[i(2\phi_0-\phi_\alpha-\phi_{-\alpha})]\sum_{\mathbf{p},l,\sigma}1/[\epsilon_{\mathbf{p}}^2+(\pi^2l^2/\beta^2)+(gt_0/\beta)][\epsilon_{\mathbf{p}+\mathbf{Q}}^2+(\pi^2(l+m)^2/\beta^2)+(gt_0/\beta)]$$

$$\equiv(t_\alpha t_{-\alpha})^{1/2}\exp[i(2\phi_0-\phi_\alpha-\phi_{-\alpha})]\delta_\alpha(t_0). \quad (4.13)$$

Finally, the contribution of Fig. 9(c) is just the complex conjugate of (4.13); i.e., we need only reverse the signs of the phase angles. None of these stars have any rotational symmetry; therefore $W_{\mathcal{S}}=1$ for each of them.

The desired expansion of Y about the point s is

$$Y=Y(s)+\tfrac{1}{2}Y''(s)(t_0-s)^2+\sum_{\alpha\neq(0,0)}\{(1-\gamma_\alpha(s))t_\alpha+\delta_\alpha(s)\cos(2\phi_0-\phi_\alpha-\phi_{-\alpha})(t_\alpha t_{-\alpha})^{1/2}\}+\cdots. \quad (4.14)$$

We may visualize the situation as follows. The point s lies on the boundary of a many-dimensional region of integration. We wish to prove that, if we move in any direction away from s *into* this region of integration, the values of $\mathrm{Re}Y$ given by (3.17) always will increase.

First note that δ_α is real and positive. Thus the smallest values of Y will be found when

$$\cos(2\phi_0-\phi_\alpha-\phi_{-\alpha})=-1. \quad (4.15)$$

We then must examine an expression of the form

$$\mathrm{Re}(1-\gamma_\alpha)t_\alpha+\mathrm{Re}(1-\gamma_{-\alpha})t_{-\alpha}-2\delta_\alpha(t_\alpha t_{-\alpha})^{1/2}. \quad (4.16)$$

From (4.12) we can verify that

$$\gamma_{-\alpha}=\gamma_\alpha^*. \quad (4.17)$$

Next use (4.17) and complete the square in (4.16) to obtain

$$(1-\mathrm{Re}\gamma_\alpha)(t_\alpha^{1/2}-t_{-\alpha}^{1/2})^2+2(1-\mathrm{Re}\gamma_\alpha-\delta_\alpha)(t_\alpha t_{-\alpha})^{1/2}. \quad (4.18)$$

From (4.18) and the fact that δ_α is positive, we deduce that the condition for $Y(s)$ to be a minimum is

$$1-\mathrm{Re}\gamma_\alpha(s)-\delta_\alpha(s)>0. \quad (4.19)$$

According to (4.12) and (4.13),

$$\mathrm{Re}\gamma_\alpha(s)+\delta_\alpha(s)=\frac{g}{2\Omega\beta}\sum_{\mathbf{p},l,\sigma}\frac{\epsilon_{\mathbf{p}+\mathbf{Q}}\epsilon_{\mathbf{p}}+[\pi^2l(l+m)/\beta^2]+(gs/\beta)}{[\epsilon_{\mathbf{p}}^2+(\pi^2l^2/\beta^2)+(gs/\beta)][\epsilon_{\mathbf{p}+\mathbf{Q}}^2+(\pi^2(l+m)^2/\beta^2)+(gs/\beta)]}. \quad (4.20)$$

s is determined by Eq. (4.10), which can be rewritten in the form

$$1=\frac{g}{4\Omega\beta}\sum_{\mathbf{p},l,\sigma}\left\{\frac{1}{\epsilon_{\mathbf{p}}^2+(\pi^2l^2/\beta^2)+(gs/\beta)}+\frac{1}{\epsilon_{\mathbf{p}+\mathbf{Q}}^2+[\pi^2(l+m)^2/\beta^2]+(gs/\beta)}\right\}$$

$$=\frac{g}{4\Omega\beta}\sum_{\mathbf{p},l,\sigma}\frac{\epsilon_{\mathbf{p}+\mathbf{Q}}^2+\epsilon_{\mathbf{p}}^2+[2\pi^2l(l+m)/\beta^2]+(\pi^2m^2/\beta^2)+(2gs/\beta)}{[\epsilon_{\mathbf{p}}^2+(\pi^2l^2/\beta^2)+(gs/\beta)][\epsilon_{\mathbf{p}+\mathbf{Q}}^2+(\pi^2(l+m)^2/\beta^2)+(gs/\beta)]}. \quad (4.21)$$

By subtracting (4.20) from (4.21) we find

$$1-\mathrm{Re}\gamma_\alpha(s)-\delta_\alpha(s)=\frac{g}{4\Omega\beta}\sum_{\mathbf{p},l,\sigma}\frac{(\epsilon_{\mathbf{p}+\mathbf{Q}}-\epsilon_{\mathbf{p}})^2+(\pi^2m^2/\beta^2)}{[\epsilon_{\mathbf{p}}{}^2+(\pi^2l^2/\beta^2)+(gs/\beta)][\epsilon_{\mathbf{p}+\mathbf{Q}}{}^2+(\pi^2(l+m)^2/\beta^2)+(gs/\beta)]}. \tag{4.22}$$

The right-hand side of (4.22) is obviously a positive quantity, which is what we wanted to prove.

Having convinced ourselves that the point s is a local minimum of Y for temperatures below T_c, we may proceed to evaluate the partition function. When we insert (4.14) into (2.17) we find that we must evaluate products of integrals of the form

$$I_\alpha=\frac{\Omega^2}{4\pi^2}\int_0^\infty dt_\alpha\int_0^\infty dt_{-\alpha}\int_0^{2\pi}d\phi_\alpha\int_0^{2\pi}d\phi_{-\alpha}\exp\{-\Omega[(1-\gamma_\alpha)t_\alpha+(1-\gamma_{-\alpha})t_{-\alpha}+2\delta_\alpha\cos(\phi_\alpha+\phi_{-\alpha}-2\phi_0)(t_\alpha t_{-\alpha})^{1/2}]\}. \tag{4.23}$$

This integration is tedious but perfectly straightforward. The result is

$$I_\alpha=[(1-\gamma_\alpha)(1-\gamma_{-\alpha})-\delta_\alpha{}^2]^{-1}. \tag{4.24}$$

Note that (4.19) is sufficient to insure that the denominator in (4.24) never vanishes. Then

$$\frac{Z}{Z_0}=e^{-\Omega Y(s)}\left(\frac{2\pi\Omega}{Y''(s)}\right)^{1/2}\times\prod_{\alpha\neq(0,0)}[(1-\gamma_\alpha)(1-\gamma_{-\alpha})-\delta_\alpha{}^2]^{-1/2}. \tag{4.25}$$

The square root occurs in the product to correct for counting each factor twice. Finally,

$$\Psi=\Psi_0+\frac{1}{\beta}Y(s)+\frac{1}{2\beta\Omega}\sum_{\alpha\neq(0,0)}\ln[(1-\gamma_\alpha)(1-\gamma_{-\alpha})-\delta_\alpha{}^2]. \tag{4.26}$$

The first two terms on the right-hand side of (4.26) are in exact agreement with the result of Bogolyubov *et al.*[13] It is these terms which were obtained by Gaudin. The last term in (4.26) may be identified as the sum of ladder diagrams computed with quasiparticle propagators, i.e., the single particle Green's functions introduced by Gor'kov.[5] To be specific, the propagator associated with the normal contraction is, in our notation,

$$G(\mathbf{p},l)=-\frac{1}{\beta}\frac{\epsilon_{\mathbf{p}}+(i\pi l/\beta)}{\epsilon_{\mathbf{p}}{}^2+\Delta^2+(\pi^2l^2/\beta^2)}, \tag{4.27}$$

where $\Delta^2=gs/\beta$ as noted in Eq. (4.11). The anomalous Green's function is

$$F(\mathbf{p},l)=-\frac{1}{\beta}\frac{\Delta}{\epsilon_p{}^2+\Delta^2+(\pi^2l^2/\beta^2)}. \tag{4.28}$$

Thus γ_α, as given by (4.12), is the numerical contribution of a section of a ladder diagram consisting of two normal electron lines. By the same reasoning, δ_α must represent a section of a ladder consisting of two anoma-

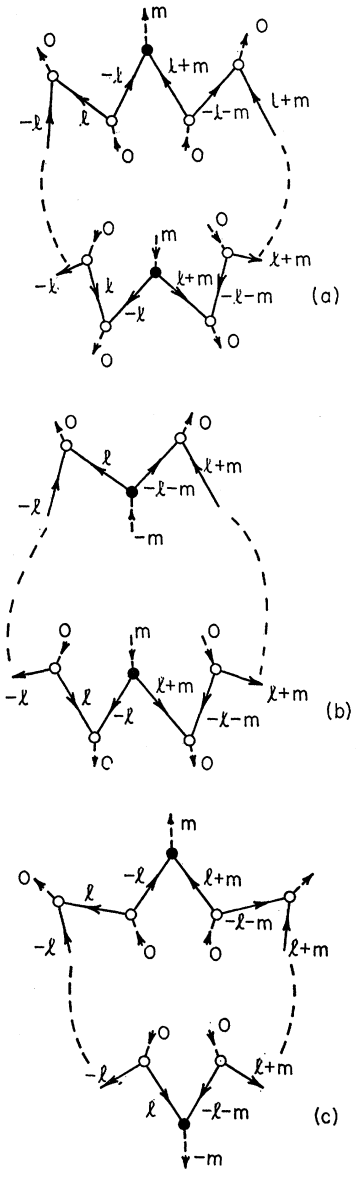

FIG. 9. The stars which determine γ_α and δ_α. The numerical values are given in Eqs. (4.12) and (4.13).

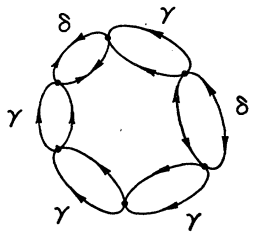

FIG. 10. A typical closed ladder consisting of normal (γ) and anomalous (δ) sections.

lous lines. A typical closed ladder containing γ_α and δ_α sections is shown in Fig. 10.

The contribution to the grand canonical potential from the sum of all closed, topologically distinct ladder diagrams constructed with only normal electron lines is

$$\frac{1}{\beta\Omega}\sum_\alpha\sum_{n=1}^{\infty}\frac{1}{n}\gamma_\alpha{}^n=-\frac{1}{\beta\Omega}\sum_\alpha\ln(1-\gamma_\alpha)$$

$$=-\frac{1}{2\beta\Omega}\sum_\alpha\ln(1-\gamma_\alpha)(1-\gamma_{-\alpha}). \quad (4.29)$$

We must complete this sum by inserting δ_α's in all possible ways. An anomalous section of a ladder diagram turns an α pair into a $-\alpha$ pair; thus we can insert only even numbers of δ_α's into any closed ladder diagram. In order to do this systematically, we construct the sum of sub-ladders of the form:

$$\delta_\alpha\gamma_{-\alpha}\cdots\gamma_{-\alpha}\delta_\alpha\gamma_\alpha\cdots\gamma_\alpha\rightarrow\delta_\alpha{}^2/(1-\gamma_\alpha)(1-\gamma_{-\alpha}).$$

Then sum all distinct, closed ladder diagrams made up of these sub-ladders:

$$\frac{1}{2\beta\Omega}\sum_\alpha\sum_n\frac{1}{n}\left[\frac{\delta_\alpha{}^2}{(1-\gamma_\alpha)(1-\gamma_{-\alpha})}\right]^n$$

$$=-\frac{1}{2\beta\Omega}\sum_\alpha\ln\left[1-\frac{\delta_\alpha{}^2}{(1-\gamma_\alpha)(1-\gamma_{-\alpha})}\right]. \quad (4.30)$$

Again, the factor $\frac{1}{2}$ corrects for overcounting in the sum over α. The sum of (4.14) and (4.15) is

$$-\frac{1}{2\beta\Omega}\sum_\alpha\ln[(1-\gamma_\alpha)(1-\gamma_{-\alpha})-\delta_\alpha{}^2], \quad (4.31)$$

which is almost in exact agreement with the last term in Eq. (4.26), the only difference being that in (4.26) we are instructed to omit the $\alpha=(0,0)$ term. Thouless[6] points out that this term makes a divergent contribution to (4.31). He correctly asserts that it may be ignored because any single term in the sum over α must be formally of order Ω^{-1}, whereas his methods are valid only to order Ω^0. [That this term must make a divergent contribution to (4.31) is implied by the fact that the right hand side of (4.22) would vanish if it were applied for $\alpha=(0,0)$.] The present theory has been constructed so as to be correct to all orders in the volume; and it is reassuring that the divergent term automatically is excluded in Eq. (4.26).

V. VELOCITY DEPENDENCE OF THE FREE ENERGY

Although the ladder-diagram contributions to Ψ given by the last terms in Eqs. (4.6) and (4.26) do not vanish like Ω^{-1}, as they should if the saddle-point method were exact, they do seem to be quite small. In the first place, the measured specific heats[14] show finite discontinuities at the transition as predicted by the Landau theory.[4] We have seen that the Landau theory is embodied in the BCS part of (4.26), i.e., the term $\beta^{-1}Y(s)$. The ladder diagrams actually produce an inverse square-root singularity; but Thouless[6] has calculated that, in order to see this anomaly experimentally, one would have to measure to within 10^{-11}°C.

A second piece of evidence in favor of the saddle-point approximation appears in some experiments related to flux quantization. Little and Parks[15] have observed that the transition temperature of a small superconducting cylinder has a periodic dependence on the applied magnetic field. More precisely, they find that the transition temperature looks like a series of well-defined scallops whose spacing is the flux quantum. The scallops are superimposed on a parabola which apparently is of macroscopic origin. This phenomenon has been analyzed in terms of conventional BCS theory by Byers and Yang.[16] In the following we shall show that such an effect is predicted by the present formalism only if we take the saddle-point picture very literally.

Rather than worry about magnetic fields and cylindrical geometries, we shall find it sufficient for our purposes simply to constrain the center of mass of the system of electrons to move with velocity $\mathbf{v}$. That is, we compute

$$Z(\beta,\mu_{\mathbf{v}},\mathbf{v})\equiv\mathrm{Tr}\exp\{-\beta(H-\mu_{\mathbf{v}}N-\mathbf{v}\cdot\mathbf{P})\}, \quad (5.1)$$

where $\mathbf{P}$ is the total momentum. Obviously $\mathbf{v}$ is equivalent to a constant vector potential, which is a reasonable approximation to the effect of a flux trapped inside a loop. This equivalent loop has a circumference equal to the side of the box in which we have imposed periodic boundary conditions. The moving system of electrons, however, seems more intuitive.

The quantities $\mu_{\mathbf{v}}$ and $\mathbf{v}$ enter Z only via the modified kinetic energies

$$\tilde{\epsilon}_{\mathbf{p}}\equiv\epsilon_{\mathbf{p}}-\mathbf{v}\cdot\mathbf{p}=p^2/2m-\mathbf{v}\cdot\mathbf{p}-\mu_{\mathbf{v}}. \quad (5.2)$$

The partition function may be taken to be a functional $Z\{\tilde{\epsilon}_{\mathbf{p}}\}$. If the system were completely free, Z would

[14] For example, see E. A. Lynton, *Superconductivity* (Methuen and Co., Ltd., London, 1962), p. 9.
[15] W. A. Little and R. D. Parks, Phys. Rev. Letters **9**, 9 (1962).
[16] N. Byers and C. N. Yang, Phys. Rev. Letters **7**, 46 (1961).

be invariant under the Galilean transformation

$$\mathbf{p}=\mathbf{p}'+m\mathbf{v}, \tag{5.3}$$

which causes

$$\tilde{\epsilon}_{\mathbf{p}}=(p'^2/2m)-\tfrac{1}{2}mv^2-\mu_{\mathbf{v}}\equiv(p'^2/2m)-\mu'=\epsilon_{\mathbf{p}'}. \tag{5.4}$$

But the set of $\mathbf{p}'$'s does not coincide exactly with the set of $\mathbf{p}$'s unless $m\mathbf{v}$ is an allowed momentum subject to the periodic boundary conditions. At least for such values of $\mathbf{v}$, however, we have

$$Z(\beta,\mu_{\mathbf{v}},\mathbf{v})=Z\{\tilde{\epsilon}_{\mathbf{p}}\}=Z\{\epsilon_{\mathbf{p}'}\}=Z(\beta,\mu',0). \tag{5.5}$$

The number of electrons is

$$\bar{N}(\mathbf{v})=\frac{1}{\beta}\frac{\partial \ln Z}{\partial\mu_{\mathbf{v}}}=-\frac{1}{\beta}\sum_{\mathbf{p}}\frac{\delta}{\delta\tilde{\epsilon}_{\mathbf{p}}}\ln Z\{\tilde{\epsilon}_{\mathbf{p}}\}$$
$$=-\frac{1}{\beta}\sum_{\mathbf{p}'}\frac{\delta}{\delta\epsilon_{\mathbf{p}'}}\ln Z\{\epsilon_{\mathbf{p}'}\}=\frac{1}{\beta}\frac{\partial}{\partial\mu'}\ln Z(\beta,\mu',0). \tag{5.6}$$

In order that $\bar{N}(\mathbf{v})=\bar{N}(0)$, we must have

$$\mu'=\mu_{\mathbf{v}}+\tfrac{1}{2}mv^2=\mu_0. \tag{5.7}$$

In a similar fashion,

$$\mathbf{P}=\frac{1}{\beta}\frac{\partial \ln Z}{\partial\mathbf{v}}=-\frac{1}{\beta}\sum_{\mathbf{p}}\mathbf{p}\frac{\delta}{\delta\tilde{\epsilon}_{\mathbf{p}}}\ln Z\{\tilde{\epsilon}_{\mathbf{p}}\}$$
$$=-\frac{1}{\beta}\sum_{\mathbf{p}'}(\mathbf{p}'+m\mathbf{v})\frac{\delta}{\delta\epsilon_{\mathbf{p}'}}\ln Z\{\epsilon_{\mathbf{p}'}\}=m\mathbf{v}\bar{N}. \tag{5.8}$$

In the last step we have used the fact that the total momentum vanishes in the system defined by $Z(\beta,\mu_0,0)$. Finally, note that the free energy is

$$F(\mathbf{v})=-\frac{1}{\beta}\ln Z(\beta,\mu_{\mathbf{v}},\mathbf{v})+\mu_{\mathbf{v}}\bar{N}+\mathbf{v}\cdot\mathbf{P}$$
$$=-\frac{1}{\beta}\ln Z(\beta,\mu_0,0)+\mu_0\bar{N}+\tfrac{1}{2}\bar{N}mv^2. \tag{5.9}$$

Presumably, Eqs. (5.5) through (5.9) are valid only on the lattice of quantized values of the momentum $m\mathbf{v}$. In the normal phase, however, these equations are certainly valid for all values of $\mathbf{v}$. This point has been emphasized by Byers and Yang.[16] To see how it works out in the present formulation, consider the quantity $\lambda_{m,\mathbf{Q}}(\mathbf{v})$ as defined by Eq. (4.1) with $\mathbf{v}$ introduced as in (5.2).

$$\lambda_{m,\mathbf{Q}}(\mu_{\mathbf{v}},\mathbf{v})=\left(\frac{1}{2\beta\Omega}\right)\sum_{\mathbf{p},l,\sigma}\frac{1}{[\epsilon_{\mathbf{p}}+\mathbf{v}\cdot\mathbf{p}+(i\pi l/\beta)][\epsilon_{\mathbf{p}+\mathbf{Q}}-\mathbf{v}\cdot(\mathbf{p}+\mathbf{Q}-i\pi/\beta)(l+m)]}. \tag{5.10}$$

For the moment assume that (5.7) describes $\mu_{\mathbf{v}}$ for all $\mathbf{v}$. This assumption is justified by the fact that (5.9) turns out to be exact; that is, the assumption does not lead to inconsistencies. If we make the transformation (5.3) in the form $-\mathbf{p}=-\mathbf{p}'+m\mathbf{v}$ and use (5.7), Eq. (5.10) becomes

$$\lambda_{m,\mathbf{Q}}(\mathbf{v})=\frac{1}{2\beta\Omega}\sum_{\mathbf{p}'=\mathbf{p}+m\mathbf{v},\,l,\sigma}\frac{1}{[\epsilon_{\mathbf{p}'}+(i\pi l/\beta)][\epsilon_{\mathbf{p}'+\mathbf{Q}-2m\mathbf{v}}-(i\pi/\beta)(l+m)]}\cong\lambda_{m,\mathbf{Q}-2m\mathbf{v}}(0). \tag{5.11}$$

The error made in the last step is no worse than that made in replacing the $\mathbf{p}$ sum by an integral. The summand is a perfectly smooth function of $\mathbf{p}$. That is, after summation over l with finite β, it has no structure within regions of order $\Delta\mathbf{p}\sim\Omega^{-1/3}$, the spacing between quantized momenta. Thus, there is no difficulty in shifting the origin in $\mathbf{p}$ space by an amount of order $\Omega^{-1/3}$ to allow for nonquantized values of $m\mathbf{v}$. It follows that (5.11) is a smooth function of $\mathbf{v}$. It is accurate to within a correction of order Ω^{-1} which also is smooth. By the same argument,

$$-\frac{1}{\beta\Omega}\ln\frac{Z(\mu_{\mathbf{v}},\mathbf{v})}{Z_0(\mu_{\mathbf{v}},\mathbf{v})}=-\frac{1}{\beta\Omega}\sum_{m,\mathbf{Q}}\ln(1-g\lambda_{m,\mathbf{Q}-2m\mathbf{v}})$$
$$=-\frac{1}{\beta\Omega}\ln\frac{Z(\mu_0,0)}{Z_0(\mu_0,0)} \tag{5.12}$$

is accurate for all values of $\mathbf{v}$. Thus, the entire $\mathbf{v}$ dependence of the free energy is contained in the term $\frac{1}{2}\bar{N}mv^2$, which is exactly what we expect for a free system of interacting electrons. In the normal phase there is no detailed structure in $F(\mathbf{v})$ induced by the imposition of boundary conditions in a fixed frame of reference.

Now let us try to repeat this argument for the superconducting phase. We have seen that, for $T<T_c$ and $\mathbf{v}=0$, the integrand in (2.17) has a maximum at the point s along the $t_{0,0}$ axis. The saddle-point picture implies that this maximum is a sharp peak such that the integrand is exponentially small along other orthogonal axes in t space. The crucial feature which we must account for now is that there are stationary points of this integrand—presumably not true maxima—along $\alpha=(0,\mathbf{Q})$ axes for nonvanishing $\mathbf{Q}$. When we vary $\mathbf{v}$ away from zero, the absolute maximum of the integrand jumps from one to another of these stationary points

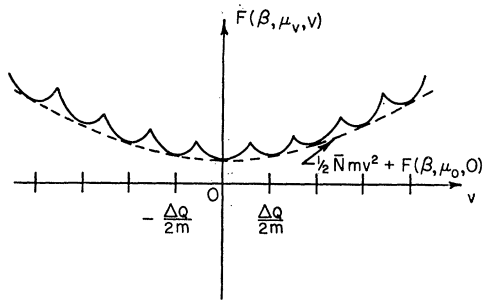

FIG. 11. The free energy F as a function of velocity in the superconducting phase.

giving rise to the discontinuous scallops in the free energy. In the normal phase the peak remained at the origin and no such behavior occurred.

Let us denote by $Y_{\mathbf{Q}}(t_{\mathbf{Q}})$ the value of $Y\{t,\phi\}$ along the $\alpha=(0,\mathbf{Q})$ axis. In exact analogy to Eq. (4.9), we have

$$Y_{\mathbf{Q}}(t_{\mathbf{Q}})=t_{\mathbf{Q}}-\frac{1}{2\Omega}\times\sum_{\mathbf{p},l,\sigma}\ln\left[1+\frac{gt_{\mathbf{Q}}}{\beta}\frac{1}{[\epsilon_{\mathbf{p}}+(i\pi l/\beta)][\epsilon_{\mathbf{p}+\mathbf{Q}}-(i\pi l/\beta)]}\right]. \tag{5.13}$$

$Y_{\mathbf{Q}}$ has a minimum at $t_{\mathbf{Q}}=s_{\mathbf{Q}}$ such that

$$\frac{g}{2\Omega\beta}\sum_{\mathbf{p},l,\sigma}\frac{1}{[\epsilon_{\mathbf{p}}+(i\pi l/\beta)][\epsilon_{\mathbf{p}+\mathbf{Q}}-(i\pi l/\beta)]+(gs_{\mathbf{Q}}/\beta)}=1. \tag{5.14}$$

This is just the gap equation which would be obtained if one chose to form Cooper pairs with total momentum $\mathbf{Q}$. The stationary point $s_{\mathbf{Q}}$ apparently corresponds to a pairing potential which generates a supercurrent. According to (5.13) and (5.14), $Y_{\mathbf{Q}}(s_{\mathbf{Q}})$ is an even function of $\mathbf{Q}$; thus, for small $\mathbf{Q}$ we may write

$$Y_{\mathbf{Q}}(s_{\mathbf{Q}})\cong Y_0(s_0)+\Upsilon Q^2. \tag{5.15}$$

The stable equilibrium state must carry zero current; therefore Υ must be positive.

Now the same discussion which led to Eq. (5.11) implies that

$$Y_{\mathbf{Q}}(s_{\mathbf{Q}},\mu_{\mathbf{v}},\mathbf{v})=Y_{\mathbf{Q}-2m\mathbf{v}}(s_{\mathbf{Q}-2m\mathbf{v}},\mu_0,0)\cong Y_0(s_0)+\Upsilon(\mathbf{Q}-2m\mathbf{v})^2. \tag{5.16}$$

To obtain the partition function for any given $\mathbf{v}$, we choose that $\mathbf{Q}$ which makes $Y_{\mathbf{Q}}$ smallest.

$$-\frac{1}{\beta\Omega}\ln\frac{Z(\mu_{\mathbf{v}},\mathbf{v})}{Z_0(\mu_{\mathbf{v}},\mathbf{v})}=-Y_0(s_0,\mu_0,0)+\frac{1}{\beta}\operatorname{Min}_{\mathbf{Q}}\Upsilon(\mathbf{Q}-2m\mathbf{v})^2. \tag{5.17}$$

The fact that each $Y_{\mathbf{Q}}$ is a smooth function of $\mathbf{v}$ again justifies our assumption concerning $\mu_{\mathbf{v}}$; but the free-energy function now has the structure mentioned above. This function is illustrated in Fig. 11. This sort of behavior of the free energy implies a similar behavior of the transition temperature. Just such a curve—even including the sharp cusps between the scallops—is seen experimentally.[15]

APPENDIX: NONSEPARABLE POTENTIALS

For purposes of completeness, we indicate here how the present analysis may be applied when the electron-electron interaction is not separable but may be expanded as a sum of separable potentials. We consider the pair model with a Hamiltonian of the form

$$H-\mu N=\sum_{\mathbf{p},\sigma}\epsilon_{\mathbf{p}}a_{\mathbf{p},\sigma}{}^{\dagger}a_{\mathbf{p},\sigma}-\frac{1}{2\Omega}\sum_{\mathbf{p},\mathbf{p}',\sigma}\Big(\sum_i v_{\mathbf{p}}{}^{(i)}v_{\mathbf{p}'}{}^{(i)}\Big)a_{\mathbf{p}\sigma}{}^{\dagger}a_{-\mathbf{p},-\sigma}{}^{\dagger}a_{-\mathbf{p}',-\sigma}a_{\mathbf{p}',\sigma}. \tag{A1}$$

It will be shown that the Gaudin approximation ($m=0$ interaction lines only) leads to the correct gap equation.

Clearly we now must consider a variety of interaction lines and points on stars labeled with indices $i,j,\cdots$, etc. In exact analogy with the derivation in Sec. II, the partition function is

$$\frac{Z}{Z_0}=\prod_i\left(\frac{\Omega}{2\pi}\int_0^{\infty}dt_i\int_0^{2\pi}d\phi_i\right)\exp[-\Omega Y\{t,\phi\}], \tag{A2}$$

where

$$Y=\sum_i t_i+\sum_{\mathcal{S}}\frac{1}{W_{\mathcal{S}}}K_{\mathcal{S}}\{t,\phi\}. \tag{A3}$$

$K_{\mathcal{S}}$ is the numerical value of the star $\mathcal{S}$ computed now with a factor $v_{\mathbf{p}}{}^{(i)}t_i{}^{1/2}\exp(i\phi_i)$ at each external i vertex and $v_{\mathbf{p}}{}^{(i)}t_i{}^{1/2}\exp(-i\phi_i)$ at each internal i vertex. Unlike the cases treated previously, $K_{\mathcal{S}}$ depends only on the number of the various vertices and not on their order. Thus, we may evaluate $K_{\mathcal{S}}$ explicitly. For combinatorial purposes it is convenient to think of an external vertex and its right neighboring internal vertex as a single entity, that is, a "point" (i,j). Let the number of (i,j) points in a star $\mathcal{S}$ be $N_{ij}(\mathcal{S})$. Then we can write

$$K_{\mathcal{S}}=\frac{1}{2\Omega}\sum_{\mathbf{p},l,\sigma}\prod_{(i,j)}(-\xi_{ij})^{N_{ij}(\mathcal{S})}, \tag{A4}$$

where

$$\xi_{ij}\equiv\frac{1}{\beta}v_{\mathbf{p}}{}^{(i)}v_{\mathbf{p}}{}^{(j)}(t_it_j)^{1/2}\times\exp[i(\phi_i-\phi_j)]\left[\frac{1}{\epsilon_p{}^2+(\pi^2l^2/\beta^2)}\right]. \tag{A5}$$

Because $K_{\mathcal{S}}$ is independent of the arrangement of the set of points $\{N_{ij}\}$, we may perform the sum over arrangements which is required in (A3). The number

of ways in which we can arrange the points along a line is

$$k!/\prod_{(i,j)} N_{ij}!, \tag{A6}$$

where k is the total number of points; i.e.,

$$k=\sum_{(i,j)} N_{ij}. \tag{A7}$$

A star is constructed by closing the ends of the line. Now a star of symmetry W will occur k/W times in this procedure. It follows that

$$\sum_{\text{arrangements}} \frac{1}{W_{\mathcal{S}}}=\frac{(k-1)!}{\prod_{(i,j)} N_{ij}!}; \tag{A8}$$

and

$$\sum_{\mathcal{S}} \frac{1}{W_{\mathcal{S}}} K_{\mathcal{S}}=\sum_{\{N_{ij}\}}{}' (k-1)!\frac{1}{2\Omega}\sum_{\mathbf{p},l,\sigma}\prod_{(i,j)}\frac{(-\xi_{ij})^{N_{ij}}}{N_{ij}!}, \tag{A9}$$

where the restriction (A7) is understood in the sum over sets $\{N_{ij}\}$.

The sums in (A9) may be performed by the same sorts of techniques which have been used throughout this paper. We first relax the restriction (A7) by inserting

$$\delta_{k,\sum_{(i,j)} N_{ij}}=\frac{1}{2\pi}\int_0^{2\pi} d\theta e^{ik\theta}\exp[-i\sum_{(i,j)} N_{ij}\theta], \tag{A10}$$

which leads to

$$\begin{aligned}\sum_{\mathcal{S}} \frac{1}{W_{\mathcal{S}}} K_{\mathcal{S}}&=\sum_k \frac{(k-1)!}{2\pi}\int_0^{2\pi} d\theta e^{ik\theta}\frac{1}{2\Omega}\\ &\quad\times\sum_{\mathbf{p},l,\sigma}\prod_{(i,j)}\sum_{N=0}^{\infty}\frac{(-\xi_{ij}e^{-i\theta})^N}{N!}\\ &=\sum_k \frac{(k-1)!}{2\pi}\int_0^{2\pi} d\theta e^{ik\theta}\frac{1}{2\Omega}\sum_{\mathbf{p},l,\sigma}\exp[-\sum_{(i,j)}\xi_{ij}e^{-i\theta}].\end{aligned} \tag{A11}$$

The θ integration is performed by making the transformation $z=e^{-i\theta}$ and integrating around the unit circle. We obtain

$$\begin{aligned}\sum_{\mathcal{S}} \frac{1}{W_{\mathcal{S}}} K_{\mathcal{S}}&=\sum_k \frac{1}{2k\Omega}\sum_{\mathbf{p},l,\sigma}(-\sum_{(i,j)}\xi_{ij})^k\\ &=-\frac{1}{2\Omega}\sum_{\mathbf{p},l,\sigma}\ln(1+\sum_{(i,j)}\xi_{ij})\\ &=-\frac{1}{2\Omega}\sum_{\mathbf{p},l,\sigma}\ln\left(1+\frac{|\Delta_{\mathbf{p}}|^2}{\epsilon_{\mathbf{p}}^2+(\pi^2l^2/\beta^2)}\right).\end{aligned} \tag{A12}$$

In the last step, we have made the suggestive identification

$$\Delta_{\mathbf{p}}=\beta^{-1/2}\sum_i v_{\mathbf{p}}^{(i)} t_i^{1/2} e^{i\phi_i}. \tag{A13}$$

The partition function is evaluated by locating the minimum of Y in t,ϕ space. Here the minimum turns out to occur in the interior of the region of integration; and we may locate it by direct differentiation. Consider first

$$\begin{aligned}\frac{\partial Y}{\partial\phi_i}&=1-\frac{1}{2\Omega}\sum_{\mathbf{p},l,\sigma}\frac{1}{\epsilon_{\mathbf{p}}^2+(\pi^2l^2/\beta^2)+|\Delta_{\mathbf{p}}|^2}\\ &\quad\times\sum_i\frac{2v_{\mathbf{p}}^{(i)}v_{\mathbf{p}}^{(j)}}{\beta}(t_it_j)^{1/2}\sin(\phi_j-\phi_i)=0.\end{aligned} \tag{A14}$$

This equation will be satisfied for all i if we set all the ϕ_i's equal to the same constant, say ϕ. As expected, the phase of Δ in (A13) is undetermined. Then

$$\frac{\partial Y}{\partial t_i}=1-\frac{1}{2\Omega}\sum_{\mathbf{p},l,\sigma}\frac{1}{\epsilon_{\mathbf{p}}^2+(\pi^2l^2/\beta^2)+|\Delta_{\mathbf{p}}|^2}\frac{v_{\mathbf{p}}^{(i)}e^{-i\phi}}{\beta^{1/2}t_i^{1/2}}\Delta_{\mathbf{p}}=0. \tag{A15}$$

If we multiply (A15) by

$$\beta^{-1/2}v_{\mathbf{p}}^{(i)}t_i^{1/2}e^{i\phi}$$

and sum over i, we find

$$\begin{aligned}&\beta^{-1/2}\sum_i v_{\mathbf{p}}^{(i)}t_i^{1/2}e^{i\phi}\\ &\quad=\Delta_{\mathbf{p}}=\frac{1}{2\Omega\beta}\sum_{\mathbf{p}',l,\sigma}\sum_i\frac{v_{\mathbf{p}}^{(i)}v_{\mathbf{p}'}^{(i)}\Delta_{\mathbf{p}'}}{\epsilon_{\mathbf{p}'}^2+(\pi^2l^2/\beta^2)+|\Delta_{\mathbf{p}'}|^2},\end{aligned} \tag{A16}$$

which is exactly the BCS gap equation for a sum of separable potentials.