VI. CONCLUSIONS

It is clear that, even allowing the approximations made, the argument presented is at best a formal one. To justify the differentiations performed the series differentiated must converge uniformly whereas the series in question are known not to converge (or, in fact, exist) at all unless a partial summation of the diagonal matrix elements is first performed. On the other hand, the argument makes the result plausible and shows the arrangement in which terms must be taken to obtain a consistent theory.

The neglect of the S linked terms and the overlapping vertex terms is probably of greater physical interest. It may be possible to take the two effects into consideration simultaneously but if this is the case the correct accounting procedure to be followed is by no means clear. The S linked terms have been shown by Sawada[5] to give rise to the effect termed by other authors[1] the depletion effect. Therefore, neglecting the S linked terms is equivalent to neglecting the depletion effect and is, therefore, perhaps justifiable at low densities only.

The chief interest of this theory may be the fact that it allows a consistent approach to the problem of a bound, but saturated, many-boson system, i.e., liquid helium. The theories of the many-boson system which have been developed all are limited to repulsive forces. The reason is essentially that if the forces are attractive so as to provide a bound state, $\tilde{v}(0)$ is negative. The state in which all particles have zero momentum is then no longer the ground state of the diagonal part (in momentum representation) of the Hamiltonian and so cannot lead to the perturbed ground state. One reflection of this is that the lowest order phonon spectrum becomes imaginary.

It is seen that this difficulty may be avoided in practice for liquid helium by considering densities large enough that the energy versus density curve is concave upwards. The single-particle energies are then positive despite the fact that the ground-state energy is negative and a consistent theory may be obtainable. One need not be overly concerned about neglecting low densities since the system cannot exist stably at a density below the equilibrium density in any event.

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Analytic Properties of the Partition Function near the Normal-to-Superconducting Phase Transition*

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It is shown that the grand partition function for a superconductor has analytic properties near the transition point in the complex temperature plane similar to those described by Lee and Yang in their statistical theory of condensation. The normal and superconducting regions of the complex plane are separated by a line of zeroes which, in the limit of infinite volume, becomes a natural boundary.

THE purpose of this note to point out that an expression for the grand partition function for a superconductor, originally derived by Gaudin,[1] has analytic properties near the transition point in the complex temperature plane similar to those described by Lee and Yang[2] in their statistical theory of condensation.

The Lee-Yang analysis pertains to a classical system of hard-core molecules. Only a finite number of such molecules will fit into a volume Ω; and it follows from this that the grand partition function Z is an entire function of the fugacity y. Z must have a finite number of zeroes distributed symmetrically about the real axis in the complex y plane. None of these zeroes can occur on the real, positive y axis; but as the volume tends to infinity, the zeroes may cluster densely on lines crossing this axis, thus pinching it at some points. Lee and Yang identify such points as phase transitions.

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* Supported in part by the National Science Foundation.
[1] M. Gaudin, Nucl. Phys. **20**, 513 (1960).
[2] C. N. Yang and T. D. Lee, Phys. Rev. **87**, 404 (1952); T. D. Lee and C. N. Yang, *ibid.* **87**, 410 (1952).

We wish to consider the quantum system described by the BCS pair Hamiltonian[3]

$$H-\mu N=\sum_{\mathbf{p},\sigma} \epsilon_{\mathbf{p}} a_{\mathbf{p},\sigma}{}^{\dagger} a_{\mathbf{p},\sigma} -\frac{g}{2\Omega} \sum_{\substack{\mathbf{p},\mathbf{p}',\sigma \\ -\epsilon_M<\epsilon_{\mathbf{p}},\epsilon_{\mathbf{p}'}<\epsilon_M}} a_{\mathbf{p},\sigma}{}^{\dagger} a_{-\mathbf{p},-\sigma}{}^{\dagger} a_{-\mathbf{p}',-\sigma} a_{\mathbf{p}',\sigma}. \quad (1)$$

Here the $\epsilon_{\mathbf{p}}$'s are kinetic energies measured from the chemical potential μ. Ω is the volume and g is a coupling constant which is positive for attractive interactions between pairs of electrons in a band of width $2\epsilon_M$. Obviously, (1) does not satisfy the criteria for the Lee-Yang analysis. In particular, there are no hard cores to provide an upper bound for the density, which is essential to the argument concerning discrete zeroes in the complex y plane. The Pauli principle, however, does provide a mechanism which forces states of high density to have high energies, thus making them statistically less important in the grand canonical ensemble. It seems possible, therefore, that the Lee-Yang picture is of quite general validity.

According to the above argument, no truncation of the conventional linked cluster expansion can describe a phase transition because any such truncation violates the Pauli principle. For example, the sum of ladder diagrams[4] cannot be continued analytically from above to below the transition temperature, nor can the BCS solutions be continued in the other direction. A much more complete and detailed solution of the many-body problem is required, allowing, in particular, a study of Z for large but finite volume.

The basic ingredient of such a solution is contained in the work of Gaudin.[1] After an ingenious diagrammatic rearrangement of the standard perturbation expansion, 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 the transition temperature. These techniques recently have been generalized and extended by one of the present authors (J.S.L.); and a detailed report of this work is now in preparation. Here we shall present only the particular result which is relevant to this discussion.

Gaudin's expression for the grand partition function may be written in the form,

$$\frac{Z}{Z_0}=\Omega\int_0^{\infty} dt\, \exp[-\Omega Y(t,\beta)], \quad (2)$$

where Z_0 is the partition function for the noninteracting system and

$$Y(t,\beta)=t-\frac{2}{\Omega}\sum_{\mathbf{p}} \ln\left\{\frac{\cosh[\frac{1}{2}\beta(\epsilon_{\mathbf{p}}{}^2+gt/\beta)^{1/2}]}{\cosh(\frac{1}{2}\beta\epsilon_{\mathbf{p}})}\right\}. \quad (3)$$

[3] J. Bardeen, L. N. Cooper, and J. R. Schrieffer, Phys. Rev. **108**, 1175 (1957).

[4] D. J. Thouless, Ann. Phys. (N. Y.) **10**, 553 (1960).

The recent, more rigorous, analysis indicates that this expression for Z is correct apart from factors of order unity. Thus, as shown by Gaudin, Eq. (2) yields the correct grand canonical potential,

$$\psi(\beta)=-\frac{1}{\beta\Omega}\ln Z, \quad (4)$$

for both normal and superconducting phases in the limit $\Omega\rightarrow\infty$. The detailed analytic properties of (2) turn out to be exactly correct in the very immediate vicinity of the transition point, which is, of course, the most interesting place.

We are looking only for qualitative agreement with Lee and Yang; therefore, it does not make much difference which variable we choose for analytic continuation of Z. It is slightly more convenient to continue in the inverse temperature β. We shall perform this continuation by means of a saddle-point analysis of (2).

First note that the singularities of $Y(t,\beta)$, given by

$$\epsilon_{\mathbf{p}}{}^2\beta^2+gt\beta+(2n+1)^2\pi^2=0, \quad (5)$$

lie outside the region $\mathrm{Re}t\geq 0$, $\mathrm{Re}\beta>0$; thus, the only singularities of $\psi(\beta)$ in the half-plane $\mathrm{Re}\beta>0$ are branch points lying at the zeroes of Z.

When β is fixed at a real value less than the critical inverse temperature β_c, Y increases monotonically as t varies from 0 to $+\infty$. For $\beta>\beta_c$, Y has a single minimum at $t=s>0$. The critical temperature $\beta_c{}^{-1}$ occurs when the minimum s passes through $t=0$, and is thus the solution of

$$Y_t(0,\beta_c)=0. \quad (6)$$

(Here we use subscripts to denote partial derivatives of Y with respect to t, β.) Then, for a fixed complex value of β in the vicinity of β_c, Y has a saddle point s near the origin, the position of which is determined as a function of β by

$$Y_t(s,\beta)=0. \quad (7)$$

Equation (7) turns out to be the usual B.C.S. gap equation. It may be expanded about β_c to give

$$s=-\frac{Y_{t,\beta}(0,\beta_c)}{Y_{t^2}(0,\beta_c)}(\beta-\beta_c)+\cdots. \quad (8)$$

One may check from Eq. (3) that all of the required derivatives exist and that $Y_{t,\beta}<0$, $Y_{t^2}>0$.

A contour map of the surface $\mathrm{Re}Y(t,\beta)$ in the complex t plane for fixed β is shown in Fig. 1. The dominant contribution to Z for large Ω depends on the position of the origin 0 relative to the saddle-point s. If 0 lies either on a mountain or in the valley (a), we always may find a path of integration from 0 to $+\infty$ along which the modulus of the integrand decreases monotonically. In this case Z may be obtained by integrating along the path of steepest descent away from 0. We call this path

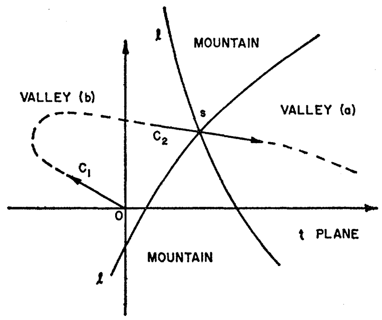

FIG. 1. Contour map of ReY in the complex t plane.

C_1, and the resulting integral Z_1:

$$\frac{Z_1}{Z_0}\approx\frac{1}{Y_t(0,\beta)}\left[1-\frac{Y_{t^2}(0,\beta)}{\Omega Y_t^2(0,\beta)}+\cdots\right]. \quad (9)$$

On the other hand, if 0 lies in the valley (b), the main contribution to Z is Z_2, the integral along the path C_2 which crosses the saddle point s.

$$Z_2/Z_0\approx\exp[-\Omega Y(s,\beta)][2\pi\Omega/Y_{t^2}(s,\beta)]^{1/2}. \quad (10)$$

In both cases $Z(\beta)$ has no zeroes and $\psi(\beta)$ is analytic.

The interesting situation occurs when 0 lies very near the level line l which separates the two cases discussed above. This happens when β lies near the line l' on which

$$\mathrm{Re}Y(s,\beta)=\mathrm{Re}Y(0,\beta)=0,\quad \mathrm{Re}(\beta-\beta_c)>0 \quad (11)$$

in the complex β plane. This line is shown in Fig. 2. Now both contours C_1 and C_2 make comparable contributions to (2); thus

$$Z\approx Z_1+Z_2. \quad (12)$$

Because Z_2 is a rapidly oscillating function of β, Z will have zeroes in the β plane along the line l'' defined by

$$|Z_1|=|Z_2|;$$

that is:

$$\mathrm{Re}Y(s,\beta)=\frac{1}{2\Omega}\ln\left\{\frac{2\pi\Omega|Y_t(0,\beta)|^2}{|Y_{t^2}(s,\beta)|}\right\},\ \mathrm{Re}(\beta-\beta_c)>0. \quad (13)$$

The position of the zeroes along this line is given by

$$\arg Z_2=\arg Z_1+(2n+1)\pi;$$

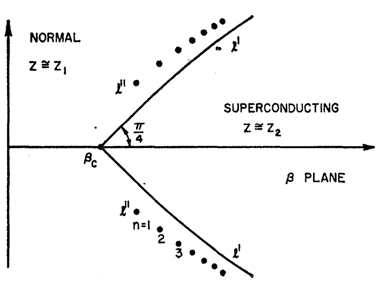

FIG. 2. Zeroes of Z in the complex β plane.

which implies

$$\mathrm{Im}Y(s,\beta)$$
$$=-\frac{1}{\Omega}[(2n+1)\pi-\arg Y_t(0,\beta)+\tfrac{1}{2}\arg Y_{t^2}(s,\beta)]. \quad (14)$$

Equations (13) and (14) may be solved explicitly by expansion about $\beta=\beta_c$. In lowest order we use Eq. (8) and define

$$-\frac{Y_{t,\beta}(0,\beta_c)}{[2Y_{t^2}(0,\beta_c)]^{1/2}}(\beta-\beta_c)\equiv\rho e^{i\theta}. \quad (15)$$

Then Eqs. (13) and (14) reduce to

$$\theta\cong\pm[\tfrac{1}{4}\pi+(1/4\Omega\rho^2)\ln(4\pi\Omega\rho^2)], \quad (16)$$

and

$$\rho^2\cong(\pi/\Omega)(2n-\tfrac{1}{4}), \quad (17)$$

when n is a large positive integer.

The above treatment breaks down for values of $\beta-\beta_c$ of order $\Omega^{-1/2}$ or less, for which the correction terms in (9) become important. The contributions from the integrations along C_1 and C_2 no longer can be separated; and the zeroes of Z very close to β_c are then found to be the solutions of

$$\mathrm{erf}(\rho e^{i\theta}\Omega^{1/2})=-1. \quad (18)$$

Even for the roots of (18) closest to $\rho=0$, Eqs. (16) and (17) locate the zeroes of Z quite accurately.

As shown in Fig. 2, the locus l'' of the zeroes of Z separates the normal and superconducting regions of the β plane. When Ω increases, l'' tends to l' [Eq. (11)], and the zeroes move toward β_c. As $\Omega\to\infty$, ψ has finite limits in both regions, but these limit functions no longer are analytic continuations of each other.

There are, in fact, a few significant differences between the above analysis of the superconducting transition and the cases studied by Lee and Yang. Instead of being orthogonal to the real axis, the natural boundary l' has a singular point at $\beta=\beta_c$, where it has the slope $\pm\frac{1}{4}\pi$. In addition, it follows from Eq. (17) that the density of zeroes, that is their number per unit length divided by Ω in the limit $\Omega\to\infty$, tends to zero like $|\beta-\beta_c|$ as $\beta\to\beta_c$. As shown by Lee and Yang, the behavior of this density is related to the nature of the transition which is here of second order.

The above analysis was based only on the form of (2) and some simple properties of Y. In the complete version of this theory the right-hand side of (2) becomes a multidimensional integral; but the saddle-point feature persists. Whenever the partition function may be represented in this form, there must exist Lee-Yang zeroes near the contour defined by Eqs. (7) and (11).