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Foundations of a comprehensive theory of liquid ^{4}He

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A theory of liquid ^{4}He is formulated that incorporates the principal elements of approaches found most successful in the past. It is grounded in quantum-mechanical correlated-basis-function formalism, which produces an elementary-excitation model for the flowing liquid. Standard statistical-mechanical techniques are used to derive explicit formulas for thermodynamic and hydrodynamic properties that are relevant to the macroscopic two-fluid equations. An important feature of this work is that it produces an explicit formula for the Lagrangian used by Zilsel to derive the two-fluid equations from a variational principle. The general formulas developed here take into account effects of interactions and constraints involving elementary excitations. It is demonstrated that temperature-dependent energy levels occur in ordinary statistical-mechanical formulas as a consequence of interactions. The fact that energy widths of elementary excitations do not enter the formulas is discussed. The formulas are applied to some simple models, and they are used there in a detailed study of the specific heat. Temperature and flow dependence of thermodynamic variables are exhibited in graphical form. It is observed that the Helmholtz potential has a peculiar behavior, and the possibility that this is connected with the changing flow properties at T_λ is studied within the context of a stability analysis involving general thermodynamic criteria. That same potential suggests that a state of flow may be thermodynamically preferred over the rest state for a range of temperatures reaching somewhat below T_λ. This is one factor that motivates a calculation of properties of quantized vortices in the liquid in the final section of the paper.

I. INTRODUCTION

The extraordinary character of liquid ^{4}He has generated problems challenging physicists for more than two-thirds of a century. Considerable progress in explaining the observed behavior has been made by applying a great variety of theoretical techniques and formalisms, many of which were developed for this specific purpose. But there are still some basic properties of liquid ^{4}He that are not well understood at a fundamental level even though substantial theoretical effort has been concentrated there for about 40 years; so major problems remain to be solved. Now it would appear to be highly useful to consolidate and extend the existing theory by adopting a single point of view and using a formalism which incorporates the principal elements of the approaches that have been most successful quantitatively. That is the goal here.

The methods and results of this paper are brought into focus in the following discussion, which also explains the main connections with earlier work.

The theory here is based on a microscopic, correlated-basis-function (CBF) description of the liquid when a field of flow is present. In a direct sense it is an extension of certain work of Feynman[1,2] and of Feenberg and Jackson,[3-5] but results found by a multitude of workers support it. Of particular importance in this regard are extensive calculations[6-17] in CBF theory which account for experimentally determined properties of liquid ^{4}He with at least moderate accuracy. In this treatment, the existence of a Bose-Einstein condensate is irrelevant; without modification the theory can accommodate conditions where a condensate is either present or absent. That feature is noteworthy because recent neutron-scattering experiments indicate that the condensate fraction in superfluid ^{4}He is no more than a few percent,[18-23] and the experiments have given no indisputable evidence that there is any condensate at all.[23] The CBF formalism yields an elementary excitation model for the liquid, which may be flowing.

In the literature, the most general forms of the hydrodynamic equations of motion, associated with the well-known two-fluid model, have been derived at a phenomenological level by two distinct methods. One is Khalatnikov's[24] extension of Landau's[25] method based on Galilean invariance. The other is Zilsel's[26,27] method based on a Lagrangian. Zilsel's method is easy to apply, and it has the advantage that it does not involve intricate verbal arguments as the other one does. The results derived in the two treatments largely parallel each other, and they are valid for small as well as large flow velocities. Khalatnikov has supported the first approach with a microscopic theory based on a Boltzmann equation for elementary excitations. However, his theory does not take into account the effect of interactions of excitations in shifting the energy levels, and it seems likely that this will seriously restrict the ranges of velocity and temperature where the theory can be trusted. On the other hand, the microscopic theory in Sec. II of this paper contains the first derivation of explicit formulas for all thermodynamic and hydrodynamic properties involved in Zilsel's treatment, and it takes into account interactions of elementary excitations in such a way that it may be applicable over the entire ranges of velocity and temperature that are of most interest physically. The need for a theory that is valid even at high velocities has become more obvious since Schofield's[28] recent work in which critical velocities for superfluid flow through micron-size orifices were observed to be as high as 10 m sec^{-1}. Of course, high-fluid velocities are also associated with quantized vortices and with rapidly moving ions in liquid ^{4}He.

The theory provides a rigorous justification for the use of temperature-dependent energy levels in ordinary statistical-mechanical formulas for models in which the momentum and energy eigenvalue spectra are characteristic of a set of interacting excitations. Bendt, Cowan, and Yarnell[29] demonstrated the usefulness of such a formalism many years ago by introducing temperature-dependent energy levels extracted directly from neutron-scattering experiments. However, the procedure has not been completely justified before, although thermal Green's-function formalism[30] and thermodynamic perturbation theory[31] lend some theoretical support to the main idea. The statistical-mechanical formulas do not involve energy widths, and so they are applicable in unaltered form even at high temperatures, e.g., above the λ point, even though standard Green's-function formalism may assign large widths to the spectral function of the excitations there. An explanation of this point is given at the end of Sec. II. This result is important because since the original work of Landau,[25] it seems to have been generally believed that an elementary excitation model would be of no practical use at temperatures as high as T_λ. That belief was presumably based on uncertainty principle arguments originally, and it seemed to be reinforced by inferences drawn from thermal Green's-function theory and from line broadening observed[32-34] in neutron scattering from liquid ^{4}He in a temperature range extending somewhat below T_λ.

If there exists an upper limit on the number of excitations in the liquid, then an inequality constraint must be imposed in the statistical-mechanical formalism. A method of dealing with this condition is described near the end of Sec. II, and possible effects of such a constraint on thermodynamic properties, especially the specific heat, are examined in the latter part of Sec. III.

Section III contains a study of the dependence of thermodynamic and hydrodynamic properties of the liquid on temperature and flow velocity. Results are presented in graphical form. Early in Sec. III, attention is focused on the peculiar behavior of the Helmholtz free energy. Isotherms of this thermodynamic potential plotted versus flow velocity undergo a qualitative change at a certain temperature, the temperature where normal fluid density equals the total density when the superfluid and normal fluid are stationary. This provides a connection with the condition that Landau associated with the superfluid transition. The isotherms exhibit clearly properties that Feynman described qualitatively many years ago. The reason for the change in the flow properties of the liquid at that particular temperature is investigated by applying stability criteria within the context of general thermodynamic theory. Connections of this study of stability with work of Hohenberg and Martin[35] and Feynman[1] are pointed out. In the last half of Sec. III, the effects of interactions among elementary excitations are examined for specific models. It is found that those models are unable to account for the logarithmic behavior of the specific heat if the system remains stationary and homogeneous. In part, this provides the motivation for studying, in Sec. IV, the possibility that the liquid does not remain stationary and that quantized vortices form spontaneously in liquid ^{4}He in some range of temperature that starts below T_λ. The peculiar behavior of the thermodynamic potential mentioned earlier also suggests this possibility.

In Sec. IV the energy and size of cores of quantized vortices are calculated approximately, and the results are used in the calculation of the free energy of certain vortex arrays. If vortex arrays have lower free energy than the stationary liquid when the walls of the container are at rest, then vortices should be generated by thermal excitation alone. Taken at face value, the calculations indicate that the stationary liquid has lower free energy. However, it is pointed out that because certain approximations are made and because other arrays may have lower free energy than those examined, the results should not be regarded as conclusive. When all uncertain factors are taken into account, the calculated results are such that it seems reasonable to speculate that vortices are thermally excited in liquid ^{4}He at temperatures reaching below T_λ. This points to the possibility that the logarithmic behavior of the specific heat may be associated with rearrangement of vortices. It is conjectured that this is the mechanism which links the change in the flow properties with the specific-heat anomaly at T_λ.

Viewed in perspective, perhaps the most distinctive feature of the theory here is that it translates the rather vague, qualitative concepts of an adiabatic transformation of an isolated ground state, and a macroscopic quantum state[36] into an operational prescription for calculating the properties of liquid ^{4}He if one interprets the coordinate space representative of the macroscopic quantum state as the correlation function that includes flow in the CBF theory. That correlation function also provides a realization of the "background" in an elementary excitation theory of the two-fluid equations.

II. MICROSCOPIC BASIS OF THE TWO-FLUID EQUATIONS

Consider a system composed of N ^{4}He atoms, each of mass m, contained in a volume V, and suppose that periodic boundary conditions are imposed. The results of several existing quantum-mechanical calculations indicate that to good approximation the wave functions for elementary excitation states can be written in the product form

$$\psi(\vec{r}_1, \vec{r}_2, \ldots, \vec{r}_N) = F(\vec{r}_1, \vec{r}_2, \ldots, \vec{r}_N) \times \psi_0(\vec{r}_1, \vec{r}_2, \ldots, \vec{r}_N), \qquad (1)$$

where $\vec{r}_i$ gives the spatial position of the ith atom. F is a model function, and is different for different states of the system. The correlation function ψ_0 is a common factor in the entire set of wave functions, which is assumed to be complete. We shall be interested in the case where ψ_0 is the true ground-state wave function for the system at rest, and belongs to the energy eigenvalue E_0. A first approximation for the function F associated with a single excitation[1] is

$$F_0 = \rho_{\vec{k}} = \sum_l \exp(i\vec{k}\cdot\vec{r}_l), \qquad (2)$$

and the corresponding energy formula is $\epsilon(k) = \hbar^2 k^2/2mS(k)$, where $S(k)$ is the liquid-structure function for $T = 0$ °K. More accurate forms for F and the energy for a single excitation have been found by applying variational[6] and perturbation[4,5,16] procedures. Feynman[1] pointed out that one could find approximate forms of F for multiply excited states by using wave packets. Feenberg and Jackson solved that same problem by explicitly diagonalizing the dominant terms associated with low excitation levels in the Hamiltonian matrix.[3,5,13] These calculations also yield explicit approximate formulas for the multiple-excitation spectrum, of course. The microscopic theory is still subject to improvement; for example, the most accurate calculated values[16] for $\epsilon(k)$ do not coincide exactly with results derived from neutron-scattering experiments.[37] Also the microscopic calculations for the multiple-excitation states and energies are not as accurate as the best results for the single-excitation properties. Therefore, rather than confining our attention to particular approximate results, it seems more useful to abstract certain general properties from these calculations and to rely partly on experiment for input to our theory. Proceeding in that spirit, we shall usually take $\epsilon(k)$ from measurements made by inelastic neutron scattering.[37] For our purposes here, it is not necessary to assume specific approximate formulas for F. But using them as guides, we shall assume that each F contains no gradient operators, that it is symmetrical in the particle coordinates, and that it satisfies the specified boundary conditions. We shall be concerned with a class of models for which the momentum and energy eigenvalues, measured in the same reference frame as E_0 and ψ_0, are of the form

$$\vec{P} = \sum_i n_i \vec{p}_i \qquad (3)$$

and

$$E = E_0 + \sum_i n_i \epsilon_i + \frac{1}{2N} \sum_{i,j} f_{ij} n_i n_j + \frac{1}{3N^2} \sum_{i,j,k} f_{ijk} n_i n_j n_k + \frac{1}{4N^3} \sum_{i,j,k,l} f_{ijkl} n_i n_j n_k n_l . \qquad (4)$$

In Eq. (4), the quantities f_{ij}, f_{ijk}, and f_{ijkl} are assumed to be symmetrical functions of their indices. Furthermore, only a set of representative terms are shown explicitly. The analysis which follows can be readily generalized to cover higher-index terms. The problem of evaluating the f_{ij}, etc., is discussed in Sec. III. The factors of N have been chosen so that when the sums are approximated by integrals, by introducing density-level formulas in the usual way, then each term on the right-hand side of Eq. (4) will be extensive, provided that the indexed f's are all intensive, as we shall assume. It is natural to associate the label "interacting excitation model" with the class of systems described by Eqs. (3) and (4). An important point here is that only the momentum eigenvalues are required to have a simple structure, of the type shown in Eq. (3), in order for the elementary excitation concept to be meaninfgul. Whenever the total number of excitations is very much less than the total number of particles in the system, the interaction terms in Eq. (4) will be negligible, and the usual ideas about elementary excitations are applicable. However, for highly excited states, such as are expected to be populated at and above the λ point in liquid ^{4}He, the energy eigenvalue spectrum can be much different from the simple step structure that is assumed in prototype elementary excitation models.[25]

New states of the system can be described by introducing a phase factor in Eq. (1), as indicated below[1]:

$$\psi' = F\left[\exp\left(\frac{i}{\hbar} Nm\vec{v}_s \cdot \frac{1}{N}\sum \vec{r}_l\right)\right]\psi_0 . \tag{5}$$

$Nm\vec{v}_s$ is a c number that corresponds to additional momentum in the system, and $(1/N)\sum \vec{r}_l$ is the center-of-mass coordinate. If one were to write the phase factor to the left of F, it would probably automatically be interpreted as placing the state ψ in uniform translation with velocity $\vec{v}_s$. For heuristic reasons it has been written directly in front of ψ_0, to emphasize that it may be regarded as inducing a uniform translation of ψ_0 while the excitations accounted for by F retain their identity. We shall regard it as part of the correlation function. The assumption that F contains no gradient operators implies that it commutes with the exponential factor in Eq. (5), so that the order of the factors is inconsequential mathematically. Later in this section we shall see that the translational velocity of the ground state, viz., $\vec{v}_s$, is the same as the velocity of the superfluid component in the two-fluid equations; hence the subscript s. Applying the total-momentum operator to ψ' and taking Eq. (3) into account, one finds the eigenvalues to be

$$\vec{P} = Nm\vec{v}_s + \sum n_i \vec{p}_i . \tag{6}$$

Now let us assume that the Hamiltonian operator for the system is of the general form

$$H = -\frac{h^2}{2m}\sum \Delta_i + V(\vec{r}_1, \vec{r}_2, \ldots, \vec{r}_N) , \tag{7}$$

where the potential operator V is symmetric in the particle coordinates. Applying H to ψ' of Eq. (5), using the properties for the Laplacian operating on a product of two functions, and taking into account that the momentum and energy eigenvalues are given by Eqs. (3) and (4), respectively, when $\vec{v}_s = 0$, one finds that the new energy eigenvalues are

$$E' = E + \tfrac{1}{2}Nm v_s^2 + \vec{v}_s \cdot \sum n_i \vec{p}_i \tag{8a}$$

$$= E_0 + \tfrac{1}{2}Nm v_s^2 + \vec{v}_s \cdot \sum n_i \vec{p}_i + \sum n_i \epsilon_i + \frac{1}{2N}\sum f_{ij} n_i n_j + \frac{1}{3N^2}\sum f_{ijk} n_i n_j n_k + \frac{1}{4N^3}\sum f_{ijkl} n_i n_j n_k n_l . \tag{8b}$$

Next, let us apply the statistical-mechanical formalism of the microcanonical ensemble to the flowing liquid described above. For clarity, we shall at first neglect the interactions among excitations, and deal with the simple case where the energy eigenvalues are

$$E' = E_0 + \tfrac{1}{2}Nm v_s^2 + \vec{v}_s \cdot \sum n_i \vec{p}_i + \sum n_i \epsilon_i . \tag{9}$$

The entropy of a set of independent bosons can be found from elementary counting considerations, and is given by[38]

$$S = k \sum_i \left[(1+n_i)\ln(1+n_i) - n_i \ln n_i\right] . \tag{10}$$

Let us suppose that the flow velocity is constrained to have a fixed value $\vec{v}_s$. Then one can find conditions of thermodynamic equilibrium by maximizing the entropy over the manifold of states having fixed values of total energy and total momentum. These latter two constraints may be taken into account by introducing Lagrange multipliers β and $\vec{v}_n$, and requiring that for each value of l,

$$\frac{\partial}{\partial n_l}\left(\frac{1}{k}S - \beta E' + \beta \vec{v}_n \cdot \vec{P}'\right) = 0 . \tag{11}$$

This gives

$$\ln \frac{1+n_l}{n_l} = \beta\left[\epsilon_l + (\vec{v}_s - \vec{v}_n)\cdot \vec{p}_l\right] \tag{12}$$

and

$$n_l = \frac{1}{\exp\{\beta[\epsilon_l + \vec{p}_l \cdot (\vec{v}_s - \vec{v}_n)]\} - 1} . \tag{13}$$

By a standard argument, one can establish that $\beta = 1/kT$, where T is the temperature and k is the Boltzmann constant. Later, we shall see that the Lagrange multiplier $\vec{v}_n$ may be interpreted as the velocity of the normal fluid in the two-fluid model. One can see from Eq. (11) that the procedure we have used is equivalent to minimizing the function $W(\vec{v}_s, \vec{v}_n)$ at constant $\vec{v}_s$, $\vec{v}_n$, and T, where W is defined by

$$W(\vec{v}_s, \vec{v}_n) = E' - TS - \vec{v}_n \cdot \vec{P}' . \tag{14}$$

The other variables on which W depends are T, V, and N. Thermodynamic properties of the system may be evaluated by substituting n_l from Eq. (13) into the formulas for E', S, $\vec{P}'$, etc. By carrying out a simple rearrangement of Eq. (10) and using Eq. (13), one finds that the *thermodynamic* entropy may be written

$$TS = kT \sum \ln(1+n_i) + \sum n_i\left[\epsilon_i + \vec{p}_i \cdot (\vec{v}_s - \vec{v}_n)\right] . \tag{15}$$

From Eqs. (6), (9), and (13)–(15) it follows that

$$W(\vec{v}_s,\vec{v}_n)=E_0+\tfrac{1}{2}Nmv_s^2-Nm\vec{v}_s\cdot\vec{v}_n -kT\sum\ln(1+n_l)\,. \tag{16}$$

If the variational calculation begun in Eq. (11) were carried to completion, then it would be necessary to evaluate β and $\vec{v}_n$ so that E' and $\vec{P}'$ have the fixed values specified initially. We can avoid that difficult calculation by choosing to work with the function W, where T and $\vec{v}_n$ are regarded as independent variables instead of E' and $\vec{P}'$. A basic postulate of our theory is that $W=W(\vec{v}_s;\vec{v}_n,V,T,N)$ is the thermodynamic potential for which the primary, independent variables are those shown explicitly. The special treatment of the variable $\vec{v}_s$ will be discussed shortly. Then the differential dW must be of the following form:

$$dW=-p\,dV-S\,dT-\vec{P}'\cdot d\vec{v}_n+\mu\,dN \tag{17}$$

at constant $\vec{v}_s$. With the aid of Eq. (16) one can easily verify that

$$\left(\frac{\partial W}{\partial T}\right)_{V,N,\vec{v}_n,\vec{v}_s}=-S\,, \tag{18}$$

where S is given by Eq. (10), and that

$$\left(\frac{\partial W}{\partial \vec{v}_n}\right)_{V,N,T,\vec{v}_s}=-\vec{P}'\,, \tag{19}$$

where $\vec{P}'$ is given by Eq. (6). Equations (16) and (17) shall be regarded as providing defining formulas for the pressure p and the chemical potential μ. In the present development of the theory, we shall regard $\vec{v}_s$ as a mechanical variable, rather than as a thermodynamic one. Later, in Sec. III, we will study the consequences of altering this assumption. Now, the following Legendre transform of W,

$$E'=W+TS+\vec{v}_n\cdot\vec{P}'\,, \tag{20}$$

provides a fundamental relation, viz.,

$$E'=E'(\vec{v}_s;\vec{P}',V,S,N)\,,$$

in which all of the independent thermodynamic variables are extensive. Therefore, E' is the internal energy; its differential at constant $\vec{v}_s$ is

$$dE'=-p\,dV+T\,dS+\vec{v}_n\cdot d\vec{P}'+\mu\,dN\,. \tag{21}$$

Furthermore, E' is given in integrated form by Eq. (9) when the occupation numbers satisfy Eq. (13).

Let us now turn to the question of how these results are related to the two-fluid equations. Part of the answer is well known, and we shall deal with it summarily. First, let us *define* a normal fluid density ρ_n by the relation

$$\rho_n(\vec{v}_n-\vec{v}_s)=\frac{1}{V}\sum n_l\vec{p}_l\,, \tag{22}$$

where n_l is given by Eq. (13). This is a natural extension to arbitrary velocities of the definition used by Landau[25] when the velocities are small. Next we shall *define* the superfluid density, ρ_s, by the relation

$$\rho=\rho_s+\rho_n\,, \tag{23}$$

where ρ is the mass density, given by $\rho=M/V$, with $M=Nm$. Referring to Eq. (6), let us divide by the volume V. Then the momentum per unit volume, which is the same as the mass current density, may be written

$$\vec{j}=\rho\vec{v}_s+\rho_n(\vec{v}_n-\vec{v}_s) =\rho_s\vec{v}_s+\rho_n\vec{v}_n\,. \tag{24}$$

Many years ago, Feynman[1] gave essentially this same discussion to show how two of the basic equations in the two-fluid model, Eqs. (23) and (24), could be accounted for by a microscopic theory. Next, we shall consider some further relations which demonstrate more completely the compatibility of the two-fluid model with our microscopic theory.

Zilsel[26,27] has shown that a Lagrangian density of the following form can be used with Eckart's variational principle to generate the dissipationless equations of motion for superfluid and normal-fluid components:

$$L=\rho\left[\tfrac{1}{2}xv_n^2+\tfrac{1}{2}(1-x)v_s^2-e(\rho,s,x)-\phi\right]\,, \tag{25}$$

where e is the internal energy per gram, ϕ is the potential energy of external force per gram, s is the entropy per gram, and $x=\rho_n/\rho$. The equations found by Zilsel are valid for all values of $\vec{v}_s$ and $\vec{v}_n$. The quantity ρ_s defined by Eqs. (22) and (23) can be negative under certain conditions, as will be seen in Sec. III. Therefore, the term in Eq. (25) involving $1-x$ will be negative sometimes, at least in our microscopic theory. With this in mind, we shall refer to the first two terms in Eq. (25) as the *apparent* kinetic energy density, although the qualifier was not used in the original treatment. Zilsel did not have a formula for $e(\rho,s,x)$, but he deduced that its differential is

$$de=T\,ds+\frac{p}{\rho^2}d\rho+\frac{1}{2}(\vec{v}_n-\vec{v}_s)^2dx\,. \tag{26}$$

The first two differential coefficients follow from the assumption that e is the internal energy per gram. The third coefficient was found by Zilsel after some analysis. Only the differential form (26) was needed in Zilsel's derivation of the two-fluid equations. However, we shall demonstrate that the function e whose existence he postulated can be given explicit representation by formulas derived in the microscopic theory. Having done this, we are assured that the microscopic theory is consistent with the macroscopic two-fluid model. Let us now consider the representation of e.

In ordinary, one-fluid hydrodynamics, one deals with an intrinsic internal energy function, which does not include the kinetic energy. Paralleling this, we shall subtract the apparent kinetic energy $\frac{1}{2}M_s v_s^2+\frac{1}{2}M_n v_n^2$ from E' in Eq. (9). Here, M_s and M_n are given by $M_s=\rho_s V$ and $M_n=\rho_n V$. Taking Eqs. (22)–(24) into account, one finds the intrinsic internal energy function $\overline{E}$ to be

$$\overline{E}=E_0-\tfrac{1}{2}M_n(\vec{v}_n-\vec{v}_s)^2+\sum n_i\epsilon_i\,. \tag{27a}$$

Now let

$$\overline{e}=\overline{E}/M\,, \tag{27b}$$

and

$$e_0=E_0/M\,. \tag{27c}$$

Dividing Eq. (27a) by M, we find

$$\frac{\overline{E}}{M}=\overline{e}=e_0-\tfrac{1}{2}x(\vec{v}_n-\vec{v}_s)^2+\frac{1}{M}\sum n_i\epsilon_i\,. \tag{28}$$

It is straightforward to verify that $\overline{e}$ in Eq. (28) satisfies the differential equation in (26). To do that, one may proceed as follows. First, note that $\overline{e}$ is known explicitly in terms of $\vec{v}_s$, $\vec{v}_n$, and T. There is also an implicit dependence on V, because the quantities e_0 and ϵ_i may depend on ρ, and the total mass M is held fixed. Now observe that Eq. (26) will hold if and only if the function y defined by

$$y=e-Ts-\tfrac{1}{2}x(\vec{v}_n-\vec{v}_s)^2 \tag{29}$$

satisfies the differential equation

$$dy=\frac{p}{\rho^2}d\rho-s\,dT-\tfrac{1}{2}x\,d(\vec{v}_n-\vec{v}_s)^2\,. \tag{30}$$

If the function

$$\overline{y}=\overline{e}-Ts-\tfrac{1}{2}x(\vec{v}_n-\vec{v}_s)^2 \tag{31}$$

satisfies Eq. (30) with the statistical-mechanical expressions for p, s, and x inserted on the right-hand side, then $\overline{e}$ will have the appropriate partial derivatives, given by (26), for $\overline{e}$ to represent e. To see that $\overline{e}$ does indeed have the required partial derivatives, let us first combine Eqs. (15), (22), (28), and (31), and get

$$\overline{y}=e_0-\frac{kT}{M}\sum\ln(1+n_i)\,. \tag{32}$$

It is a simple matter to find the statistical-mechanical expression for the pressure with the aid of Eqs. (16) and (17). The result may be expressed as

$$\frac{p}{\rho^2}=\frac{\partial e_0}{\partial\rho}+\frac{1}{M}\sum n_i\frac{\partial\epsilon_i}{\partial\rho}+\frac{kT}{M\rho}\sum\ln(1+n_i)\,. \tag{33a}$$

With the aid of Eq. (32), one can then show that

$$\left(\frac{\partial\overline{y}}{\partial\rho}\right)_{T,(\vec{v}_n-\vec{v}_s)^2}=\frac{p}{\rho^2}\,. \tag{33b}$$

From our earlier discussion, the statistical-mechanical formulas for s and x are already known. By using Eq. (32), one can readily compute the other derivatives of $\overline{y}$, and thereby show that $d\overline{y}$ may indeed replace dy in Eq. (30). In dealing with the microscopic theory, we have assumed that the flow velocity $\vec{v}_s$ is uniform throughout the liquid. If the properties computed there are valid, at least to good approximation, when the flow is only locally uniform, then the energy function per unit mass $\overline{e}$ will meet the necessary requirements for it to represent e in Zilsel's Lagrangian density.

Let us now derive the formula for the chemical potential, so that it will be available for future reference. From Eqs. (16) and (17), one finds

$$\mu=\left(\frac{\partial W}{\partial N}\right)_{T,V,\vec{v}_n,\vec{v}_s}$$
$$=m\left(e_0+\rho\frac{\partial e_0}{\partial\rho}+\frac{1}{2}v_s^2-\vec{v}_s\cdot\vec{v}_n+\frac{1}{V}\sum n_i\frac{\partial\epsilon_i}{\partial\rho}\right). \tag{34a}$$

By using the Euler form of the fundamental relation, viz.,

$$E'=-pV+TS+\vec{v}_n\cdot\vec{P}'+\mu N\,, \tag{34b}$$

one can solve Eq. (34b) for μ, and substitute from Eqs, (6), (9), (10), and (33a) to see that the last expression in (34a) is indeed correct. It may be worth mentioning that the chemical potential μ in Eq. (34a) is not the same as that which usually occurs in the literature. In the notation of Hohenberg and Martin, Eq. (3.11) of Ref. 35, the chemical potential in my theory corresponds to their variable ν rather than μ. Nothing fundamental is involved here; it is simply a matter of definition. Now let us introduce a Legendre transform, call it z, of the function $\overline{y}$ in Eqs. (31) and (32), as follows:

$$z=\overline{y}+p/\rho\,, \tag{34c}$$

then

$$dz=\frac{1}{\rho}dp-s\,dT-\tfrac{1}{2}x\,d(\vec{v}_n-\vec{v}_s)^2\,. \tag{34d}$$

One can then show that the exact equation for the acceleration of the superfluid, Eq. (12) on p. 129 of Ref. 27, may be written

$$\frac{D_s\vec{v}_s}{Dt} = -\vec{\nabla}(z+\phi)\,, \tag{34e}$$

where the left-hand side is the convective derivative along the trajectory of the superfluid. The variable z in Eq. (34e) above is the quantity that is usually regarded as the chemical potential. With the aid of Eqs. (32), (33a), (34a), and (34c), one can show that

$$z - \mu/m = \vec{v}_s\cdot\vec{v}_n - \tfrac{1}{2}v_s^2\,. \tag{34f}$$

It can be shown that $z = (\partial\bar{E}/\partial M)_{S,V,M_n}$ by using the thermodynamic potential $X = \bar{E} - TS - \frac{1}{2}M_n(\vec{v}_n - \vec{v}_s)^2$ and the properties of Legendre transforms.

Next let us turn to the problem involving interacting excitation, where the energy eigenvalues are given by Eq. (8b) instead of Eq. (9). The momentum eigenvalues still have the form specified by Eq. (6), and the excitations will still be treated as independent bosons. Detailed analysis indicates that under these conditions, the entropy of a homogeneous macroscopic system is still given by Eq. (10), and the analysis suggests that Eq. (10) is exact in the thermodynamic limit in this case. Only slight changes in the usual textbook derivation[38] of the entropy of a perfect gas are needed to arrive at the formula indicated. It may be worth emphasizing strongly that in applying this formula for the entropy to liquid ^{4}He, there is no gross approximation involved analogous to that made in a mean-field model of a magnetic system or a lattice gas. The condition for thermodynamic equilibrium, which may be regarded as either maximizing the entropy or minimizing the free energy W subject to the same auxiliary conditions stated earlier, is still determined by Eq. (11). Now one finds

$$\ln\frac{1+n_l}{n_l} = \beta\left(\epsilon_l + \vec{p}_l\cdot(\vec{v}_s - \vec{v}_n) + \frac{1}{N}\sum_i f_{li}n_i + \frac{1}{N^2}\sum_{i,j} f_{lij}n_in_j + \frac{1}{N^3}\sum_{i,j,k} f_{lijk}n_in_jn_k\right); \tag{35}$$

and this implies

$$n_l = \left\{\exp\left[\beta\left(\epsilon_l + \vec{p}_l\cdot(\vec{v}_s - \vec{v}_n) + \frac{1}{N}\sum_i f_{li}n_i + \frac{1}{N^2}\sum_{i,j} f_{lij}n_in_j + \frac{1}{N^3}\sum_{i,j,k} f_{lijk}n_in_jn_k\right)\right] - 1\right\}^{-1}. \tag{36}$$

For fixed values of β, $\vec{v}_s$, and $\vec{v}_n$, Eq. (36) represents a set of simultaneous equations to be solved for the occupation numbers n_l. It is clear that those solutions will depend on the temperature as well as on $\vec{v}_s$ and $\vec{v}_n$. The occupation numbers found in that way are responsible for a temperature dependence in the excitation energies that occur in the formula for the occupation numbers themselves. When the solutions to Eq. (36) are used to evaluate the quantities occurring in the right-hand side of Eq. (14), $W = W(\vec{v}_s; \vec{v}_n, V, T, N)$ is a fundamental relation expressed in terms of the same thermodynamic variables as in the noninteracting case. The thermodynamic entropy, which is given by Eq. (10) when the occupation numbers satisfy Eq. (36), may be rewritten as follows with the aid of Eqs. (10) and (35):

$$\begin{aligned} TS &= kT\sum_l\left(\ln(1+n_l) + n_l\ln\frac{1+n_l}{n_l}\right) \\ &= kT\sum_l\ln(1+n_l) + \sum_l n_l\left(\epsilon_l + \vec{p}_l\cdot(\vec{v}_s - \vec{v}_n) + \frac{1}{N}\sum_i f_{li}n_i + \frac{1}{N^2}\sum_{i,j} f_{lij}n_in_j + \frac{1}{N^3}\sum_{i,j,k} f_{lijk}n_in_jn_k\right). \end{aligned} \tag{37}$$

When (36) is combined with (6), (8b), (37), and (14), one finds the following expression for W:

$$\begin{aligned} W(\vec{v}_s, \vec{v}_n) = E_0 + \tfrac{1}{2}Nmv_s^2 - Nm\vec{v}_s\cdot\vec{v}_n - kT\sum\ln(1+n_i) \\ - \frac{1}{2N}\sum f_{ij}n_in_j - \frac{2}{3N^2}\sum f_{ijk}n_in_jn_k \\ - \frac{3}{4N^3}\sum f_{ijkl}n_in_jj_kn_l\,. \end{aligned} \tag{38}$$

If one uses Eq. (37), it is a straightforward matter to start with Eq. (38) and show that

$$\frac{\partial W}{\partial T} = -S\,. \tag{39}$$

Also from (38) and (6), one can show that

$$\frac{\partial W}{\partial\vec{v}_n} = -\vec{P}'\,. \tag{40}$$

Therefore, when the excitations interact and occupation numbers depend on T, $\vec{v}_s$, and $\vec{v}_n$ in the manner indicated by (36), the formal relations found for the noninteracting case in Eqs. (18) and (19) still hold exactly. For the interacting excitation model, we still assume the differential of W to be given by (17). Then the potential found by taking the Legendre transform of W indicated by (20) will still be the internal energy, subject to the provision that $\vec{v}_s$ be counted as a mechanical rather than as a thermodynamic variable. The differential of E' is still given by (21), and the integrated form of the internal energy is given by (8b).

To find the intrinsic internal energy $\overline{E}$ one can again subtract the apparent kinetic energy from E'. For an interacting excitation model, $\overline{E}$ is given by

$$\begin{aligned}\overline{E} &= E' - \tfrac{1}{2}M_s v_s^2 - \tfrac{1}{2}M_n v_n^2 \\ &= E_0 - \tfrac{1}{2}M_n(\vec{v}_n - \vec{v}_s)^2 + \sum n_i \epsilon_i \\ &\quad + \frac{1}{2N}\sum f_{ij} n_i n_j + \frac{1}{3N^2}\sum f_{ijk} n_i n_j n_k \\ &\quad + \frac{1}{4N^3}\sum f_{ijkl} n_i n_j n_k n_l . \end{aligned} \tag{41}$$

Proceeding as in the noninteracting case, one now finds

$$\begin{aligned}\overline{e} &= e_0 - \tfrac{1}{2}x(\vec{v}_n - \vec{v}_s)^2 + \frac{1}{M}\sum n_i \epsilon_i \\ &\quad + \frac{1}{2NM}\sum f_{ij} n_i n_j + \frac{1}{3N^2M}\sum f_{ijk} n_i n_j n_k \\ &\quad + \frac{1}{4N^3M}\sum f_{ijkl} n_i n_j n_k n_l . \end{aligned} \tag{42}$$

With the aid of (31) and (42), one gets

$$\begin{aligned}\overline{y} &= e_0 - \frac{kT}{M}\sum \ln(1+n_i) \\ &\quad - \frac{1}{2NM}\sum f_{ij} n_i n_j - \frac{2}{3N^2M}\sum f_{ijk} n_i n_j n_k \\ &\quad - \frac{3}{4N^3M}\sum f_{ijkl} n_i n_j n_k n_l . \end{aligned} \tag{43}$$

The pressure can be computed from the free energy W in Eq. (38); the result is

$$p = -\left(\frac{\partial W}{\partial V}\right)_{T,N,\vec{v}_n,\vec{v}_s}, \tag{44a}$$

and

$$\begin{aligned}\frac{p}{\rho^2} &= \frac{\partial e_0}{\partial \rho} + \frac{1}{M}\sum n_i \frac{\partial \epsilon_i}{\partial \rho} + \frac{kT}{M\rho}\sum \ln(1+n_i) \\ &\quad + \frac{1}{NM\rho}\sum\left(f_{ij} + \frac{1}{2}\rho\frac{\partial}{\partial \rho} f_{ij}\right) n_i n_j \\ &\quad + \frac{2}{N^2M\rho}\sum\left(f_{ijk} + \frac{1}{6}\rho\frac{\partial}{\partial \rho} f_{ijk}\right) n_i n_j n_k \\ &\quad + \frac{3}{N^3M\rho}\sum\left(f_{ijkl} + \frac{1}{12}\rho\frac{\partial}{\partial \rho} f_{ijkl}\right) n_i n_j n_k n_l . \end{aligned} \tag{44b}$$

Using Eqs. (43) and (44b), one can readily show that

$$\left(\frac{\partial \overline{y}}{\partial \rho}\right)_{T,(\vec{v}_n - \vec{v}_s)^2} = \frac{p}{\rho^2}. \tag{45}$$

The following results can also be readily established with the aid of Eq. (43):

$$\left(\frac{\partial \overline{y}}{\partial T}\right)_{\rho,(\vec{v}_n - \vec{v}_s)^2} = -s \tag{46a}$$

and

$$\left(\frac{\partial \overline{y}}{\partial (\vec{v}_n - \vec{v}_s)^2}\right)_{\rho,T} = -\frac{1}{2}x. \tag{46b}$$

Therefore in the presence of interactions, $\overline{y}$ given by (43) has the partial derivatives necessary for it to replace y in Eq. (30). This implies that $\overline{e}$ given by (42) may represent the intrinsic internal energy function in Zilsel's Lagrangian density,[26,27] provided that the assumption concerning local uniformity is made again.

Digressing for a moment, let us record the formula for the chemical potential of a particle when elementary excitations interact. Perhaps the easiest method of deriving it is to use Eq. (34b), together with (6), (8b), (10), and (44b). The result is

$$\begin{aligned}\mu = m\Bigg[& e_0 + \rho\frac{\partial e_0}{\partial \rho} + \frac{1}{2}v_s^2 - \vec{v}_s\cdot\vec{v}_n + \frac{\rho}{M}\sum n_i \frac{\partial \epsilon_i}{\partial \rho} \\ & + \frac{1}{2NM}\sum\left(f_{ij} + \rho\frac{\partial}{\partial \rho} f_{ij}\right) n_i n_j \\ & + \frac{4}{3N^2M}\sum\left(f_{ijk} + \frac{1}{4}\rho\frac{\partial}{\partial \rho} f_{ijk}\right) n_i n_j n_k \\ & + \frac{9}{4N^3M}\sum\left(f_{ijkl} + \frac{1}{9}\rho\frac{\partial}{\partial \rho} f_{ijkl}\right) n_i n_j n_k n_l \Bigg]. \end{aligned} \tag{47}$$

The variable z that enters the equation for the acceleration of the superfluid, Eq. (34e), may be easily computed by substituting μ from Eq. (47) into (34f).

So far, we have dealt with the theory under the assumption that the excitations are completely independent. Later we shall find that there are reasons to suppose that an upper bound may exist for the total number of excitations, or possibly just for the total number of rotons, that can be present in the liquid. It is possible to impose such an inequality constraint in the microcanonical formalism by a simple procedure, which we shall consider now. For definiteness, suppose that the constraint is just on the rotons, and that it is given in the form

$$\mathfrak{N} \equiv \sum{}' n_i \leqslant \mathfrak{N}_0 , \tag{48}$$

where the prime is a reminder that the sum is just over the rotons, and $\mathfrak{N}_0$ is a fixed number that is assumed to be known for a system of N particles. Equilibrium conditions can be found by maximizing the entropy subject to constraints on energy and momentum and on $\mathfrak{N}$. Again we shall do this by the equivalent procedure of minimizing an appropriate free-energy function. A constraint on $\mathfrak{N}$ may be imposed by introducing an additional Lagrange multiplier, which we shall take to be α. It is, in effect, a chemical potential for the rotons. Equilibrium conditions are then determined by the equation

$$\frac{\partial}{\partial n_l}(E' - TS - \vec{v}_n \cdot \vec{P} - \alpha \mathfrak{N}) = 0 . \tag{49}$$

For those excitations that are not rotons, the occupation numbers satisfy Eqs. (35) and (36). However, for rotons, a chemical potential now occurs in the formula for the occupation numbers. Explicitly,

$$\ln \frac{1+n_l}{n_l} = \beta \Big(\epsilon_l + \vec{p}_l \cdot (\vec{v}_s - \vec{v}_n) + \frac{1}{N} \sum_i f_{li} n_i + \frac{1}{N^2} \sum_{i,j} f_{lij} n_i n_j + \frac{1}{N^3} \sum_{i,j,k} f_{lijk} n_i n_j n_k - \alpha \Big) , \tag{50}$$

and

$$n_l = \Big\{ \exp \Big[\beta \Big(\epsilon_l + \vec{p}_l \cdot (\vec{v}_s - \vec{v}_n) + \frac{1}{N} \sum_i f_{li} n_i + \frac{1}{N^2} \sum_{i,j} f_{lij} n_i n_j + \frac{1}{N^3} \sum_{i,j,k} f_{lijk} n_i n_l n_k - \alpha \Big) \Big] - 1 \Big\}^{-1} . \tag{51}$$

For specified values of T, V, $\vec{v}_s$, and $\vec{v}_n$, the Lagrange multiplier α must be selected so that $\mathfrak{N}$ has the specified value when the self-consistent values of n_1 determined from (51) are substituted into (48). The occupation numbers then have a dependence on $\mathfrak{N}$ through their dependence on α. Now, in order to impose the inequality constraint given by (48), one must find that value of $\mathfrak{N}$ which produces the minimum value of

$$W = E' - TS - \vec{v}_n \cdot \vec{P}' , \tag{52}$$

when this free-energy function is evaluated with a set of occupation numbers given by (51), and subject to the condition in (48). Two possibilities exist. Either W is a relative minimum for some value of $\mathfrak{N}$, or the minimum occurs at the end point where $\mathfrak{N} = \mathfrak{N}_0$. To investigate the possibility of a relative minimum, we note from the earlier work that led to Eq. (38) that W may be written

$$W = E_0 + \frac{1}{2} N m v_s^2 - N m \vec{v}_s \cdot \vec{v}_n - kT \sum \ln(1+n_i) - \frac{1}{2N} \sum f_{ij} n_i n_j - \frac{2}{3N^2} \sum f_{ijk} n_i n_j n_k - \frac{3}{4N^3} \sum f_{ijkl} n_i n_j n_k n_l + \alpha \mathfrak{N} . \tag{53}$$

It is a simple matter to start with Eq. (53) and show that the only solution of

$$\frac{\partial W}{\partial \mathfrak{N}} = 0 \tag{54}$$

occurs when $\alpha = 0$. Equilibrium conditions therefore are given either by solutions of Eq. (51) with $\alpha = 0$, or by (51) when α is fixed so that $\mathfrak{N} = \mathfrak{N}_0$. We shall use these results later, in Sec. III, in connection with an explicit solution of Eq. (51) for a mean-field form for roton interactions.

Now that it has been shown that the thermodynamic properties can be evaluated exactly, within the context of our theory, even when interactions are present and for arbitrary temperatures and velocities, let us show that at the same time the spectral function for the excitations may have a substantial width. Applying standard formulas of temperature-dependent Green's-function theory[30] to the interacting excitation model, one has

$$G(p,t) = (1/i) \langle T [a_{\vec{p}}(t) a^{\dagger}_{\vec{p}}(0)] \rangle , \tag{55a}$$

$$G^{>}(\vec{p},t) = (1/i) \langle a_{\vec{p}}(t) a^{\dagger}_{\vec{p}}(0) \rangle , \tag{55b}$$

$$G^{>}(\vec{p},\omega) = i \int e^{i\omega t} G^{>}(\vec{p},t) \, dt , \tag{55c}$$

$$f(\omega) = 1/(e^{\beta\omega} - 1) , \tag{55d}$$

and the spectral function

$$A(\vec{p},\omega) = \frac{1}{1+f(\omega)} G^{>}(\vec{p},\omega) , \tag{56}$$

where

$$G^{>}(\vec{p}, \omega) = \frac{2\pi \sum_{m,n} e^{-\beta E_m} |\langle n| a^{\dagger}_{\vec{p}}(0)|m\rangle|^2 \delta(\omega - (E_n - E_m))}{\sum e^{-\beta E_m}}, \tag{57}$$

and $a^{\dagger}_{\vec{p}}$ is a creation operator for an elementary excitation in the momentum state $\vec{p}$. In all of these equations we have taken $\hbar = 1$. With Eqs. (8b), (56), and (57) in view, consider what happens as the temperature increases and β decreases. Eventually there will be many different states, each characterized by a set of occupation numbers $\{n_i\}_m$, for which $\exp(-\beta E_m)$ is large. Now suppose that to each of those states we add a quasiparticle with a definite momentum $\vec{p}$. That is, we increase $n_{\vec{p}}$ by one. These new states are labeled n and have energy E_n. For illustrative purposes, let us drop the last two terms in Eq. (8b). Then

$$E_n - E_m = \epsilon + \vec{v}_s \cdot \vec{p} + \frac{1}{N} \sum_{\vec{l}} f_{\vec{p}\vec{l}}\, n_{\vec{l}}\,.$$

The sets of occupation numbers $\{n_i\}_m$ will in general produce a quasicontinuum of values for the difference $E_n - E_m$. Hence the δ function in Eq. (57) will be satisfied for a variety of closely spaced values of ω for states in which each absolute squared matrix element is a positive integer and in which $\exp(-\beta E_m)$ is relatively large. Thus if $f_{\vec{p}\vec{l}}$ is not too small, the energy width of an elementary excitation as indicated by the spectral function can be large. The width generated in this way is irrelevant to the matter of evaluating accurately the thermodynamic properties of the system in the microcanonical formalism, the approach that we have taken.

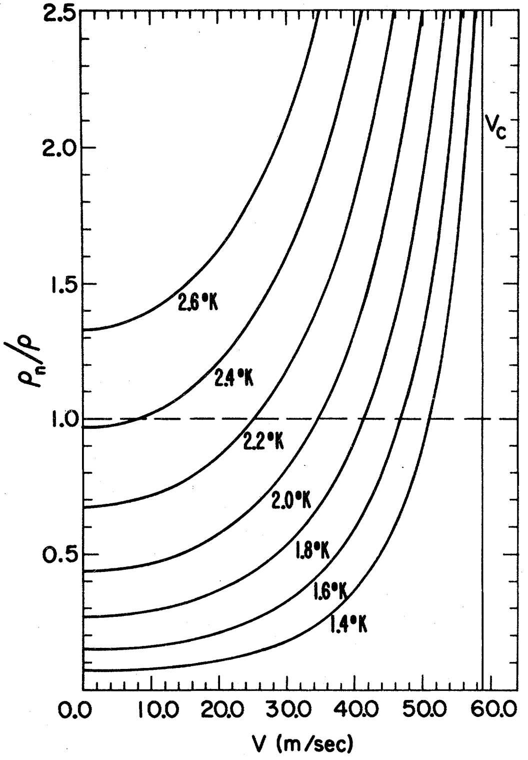

FIG. 1. Ratio ρ_n/ρ as a function of the magnitude of relative velocity $V = |\vec{v}_n - \vec{v}_s|$ for various temperatures. Normal fluid density ρ_n was computed from Eq. (22) with n_l given by Eq. (13). V_c is the Landau critical velocity. No direct interactions among excitations are present.

III. THERMODYNAMIC PROPERTIES OF LIQUID ^{4}He AT REST OR UNDER CONDITIONS OF UNIFORM FLOW

Formulas derived in Sec. II have been used to evaluate some of the thermodynamic properties of liquid ^{4}He when the flow velocity of the ground state is uniform. The velocity dependence of the normal fluid density, the number density of excitations, and the entropy per unit mass are shown in Figs. 1–3 for the model in which there are no direct interactions among excitations. In the evaluation of those functions, the elementary excitation energies were taken from the neutron scattering data for liquid ^{4}He at 1.1 °K and saturated vapor pressure as reported by Cowley and Woods.[37] The density was taken to be 0.0218 atoms Å^{-3}. All of the functions displayed in the figures diverge when the magnitude of $\vec{v}_n - \vec{v}_s \equiv \vec{V}$ approaches the Landau critical velocity from below. Neither the entropy nor the specific heat at constant volume has a discontinuity or an anomaly of any other kind at any temperature if evaluated at the system points where the velocities $\vec{v}_s$ and $\vec{v}_n$ are zero, as one expects them to be for a homogeneous liquid in a simply connected region. This behavior is evident in Fig. 4. Because the thermodynamic potential depends on the variables $\vec{v}_s$ and $\vec{v}_n$, the specific heat at constant volume is ambiguous unless one specifies two other variables that are held constant. Indicating those variables by subscripts, one can show that

$$C_{V,\vec{v}_n,\vec{v}_s} = C_{V,\vec{P}',\vec{v}_s} = C_{V,\vec{P}',\vec{Q}} = C_{V,\vec{v}_n,\vec{Q}}$$

when evaluated at $\vec{v}_n = \vec{v}_s = 0$. The common value of the specific heat at constant volume, let us call it C_V, is given by the formula

$$C_V = \frac{1}{kT^2} \sum n_i^0 (n_i^0 + 1)\, \epsilon_i^2 \,. \tag{58}$$

The variable $\vec{Q}$ is defined later in this section, immediately preceding Eq. (62). Since the specific-heat anomaly in liquid ^{4}He is of great interest, one of the main goals in our further study is

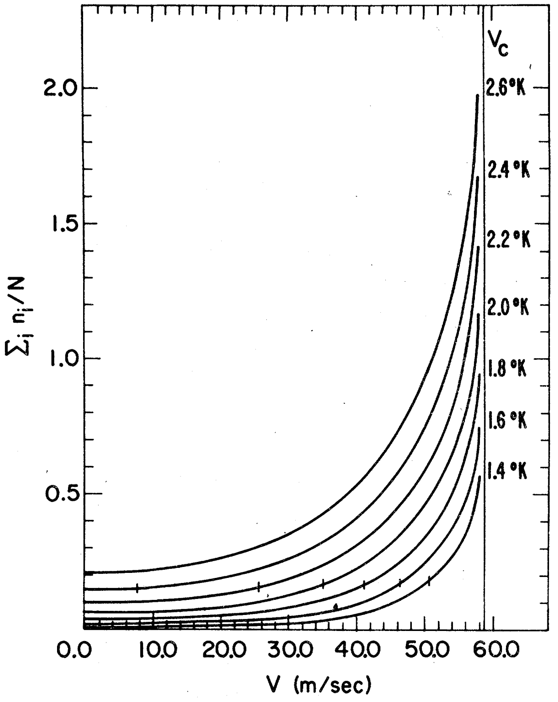

FIG. 2. Ratio of the total number of excitations to the total number of particles $\sum n_i/N$, as a function of V, where $V = |\vec{v}_n - \vec{v}_s|$. Each curve is an isotherm. No direct interactions among excitations are present, and n_i is given by Eq. (13). The short vertical line on each isotherm marks the point for which $\rho_n = \rho$.

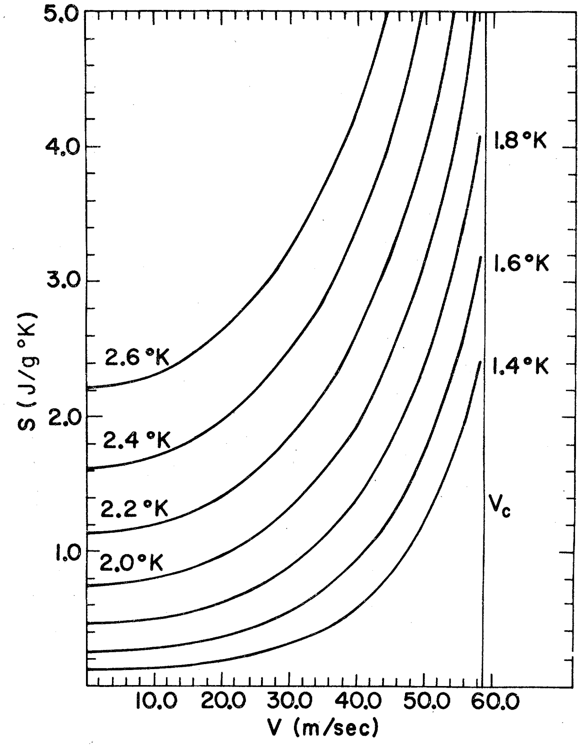

FIG. 3. Entropy per unit mass S as a function of V, where $V = |\vec{v}_n - \vec{v}_s|$. Each curve is an isotherm. No direct interactions among excitations are present. The entropy calculations were based on Eqs. (10) and (13). V_c is the Landau critical velocity.

to discover what essential feature has so far been either omitted or overlooked in the theory. Another primary objective is to explain why the flow characteristics of the liquid change at T_λ. As a first step toward those goals, let us examine the free-energy function $W(\vec{v}_s, \vec{v}_n)$ given by Eqs. (14) and (16).

For the purposes of this analysis, we shall assume that the flowing liquid is in thermodynamic equilibrium with stationary walls, and that this implies that $v_n = 0$. Under this condition, W reduces to the Helmholtz potential, as can be seen in Eq. (14); then

$$W(\vec{v}_s, \vec{v}_n = 0) = F(v_s). \tag{59a}$$

From Eqs. (16) and (59a), we get

$$F(v_s) = E_0 + \tfrac{1}{2} Nm v_s^2 - kT \sum \ln(1 + n_i). \tag{59b}$$

The free-energy per particle is shown in Fig. 5. There one can see that at constant T, the free energy tends to minus infinity at the Landau critical velocity. It seems likely that this divergence is unphysical and that a limit on the number of excitations of the same order as the number of particles in the system may determine an upper limit on the velocity range in which the curves are valid. Short vertical lines illustrate where the terminal points might be on each isotherm in Fig. 5 for an assumed value of the maximum number. For a range of low temperatures, both a relative maximum and a relative minimum are present on an isotherm. If one uses Eq. (59) in computing $\partial F/\partial v_s$ for T, V, and N held constant, and $v_n = 0$, the result is

$$\frac{\partial F}{\partial v_s} = Nm v_s + \hat{v}_s \cdot \sum n_i \vec{p}_i$$

$$= V(\rho - \rho_n) v_s. \tag{60}$$

If $\partial F/\partial v_s = 0$, then either $v_s = 0$ or $\rho = \rho_n$. With this result at hand it is clear from Fig. 5 that the maximum must occur when $\rho = \rho_n$ whenever an isotherm has two relative extrema. Feynman[36] described these qualitative features of the free energy many years ago. The calculated value of the temperature at which the maximum merges with the relative minimum is 2.415 °K. In his classic work on superfluid ^{4}He, Landau[25] suggested that the superfluid transition is associated with the condition $\rho_n = \rho$ when the liquid is at rest, a condition which is now seen to occur when a free-energy isotherm

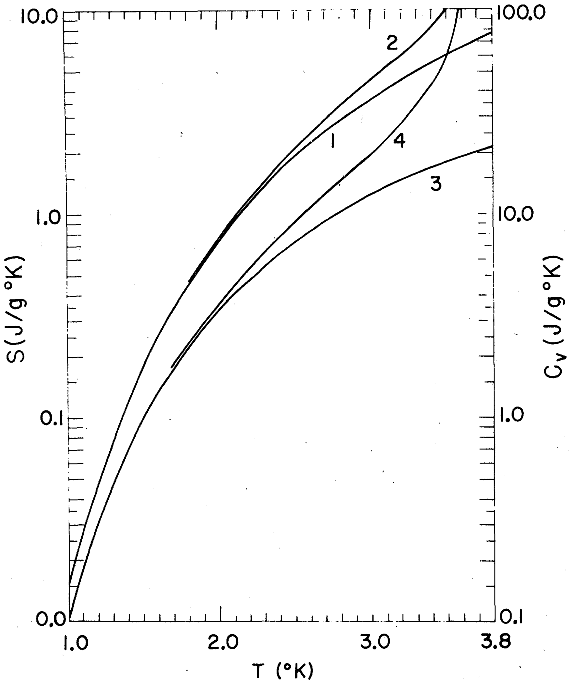

FIG. 4. Curves 1 and 2: The entropy per unit mass S as a function of temperature, for $V=|\vec{v}_n-\vec{v}_s|=0$. Curve 1 is for noninteracting excitations and curve 2 is for a mean-field interaction with $\gamma=0.2$. The values of S were computed with the aid of Eq. (10). Curves 3 and 4: The specific heat at constant volume C_V as a function of temperature, for $V=|\vec{v}_n-\vec{v}_s|=0$. Curve 3 is for noninteracting excitations and curve 4 is for a mean-field interaction with $\gamma=0.2$. V_c is the Landau critical velocity. C_V was computed from curves 1 and 2 by using finite differences.

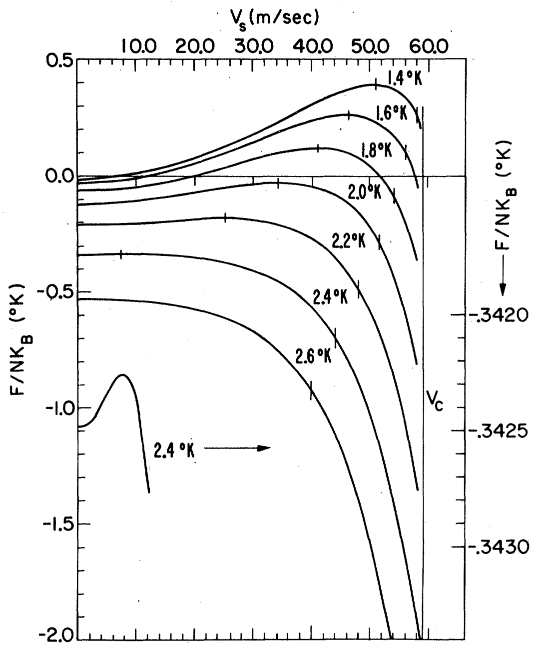

FIG. 5. Free energy per particle as a function of superfluid velocity v_s when $v_n=0$. Each curve is an isotherm. No direct interactions among excitations are present, and the calculated free energy is based on Eq. (58b), but E_0 has been subtracted out of that formula. The vertical line nearest $v_s=0$ marks the maximum on each isotherm; the other vertical line marks the point where $\sum n_l/N=0.5$. V_c is the Landau critical velocity.

undergoes a qualitative change in form. We shall call the temperature there T_λ. There may be a causal connection between these phenomena, so let us examine the situation more closely.

It is reasonable to ask first whether the formulas for the free energy and the two-fluid equations are meaningful under conditions where $\rho_n>\rho$, or said another way, when $\rho_s<0$. From what was said earlier, it is clear that $\rho_s<0$ above T_λ and for large velocities beyond the maximum on each isotherm below T_λ. Perhaps these regions can be directly excluded as physically attainable states in the theory by imposing a constraint of the form $\rho_n\leqslant\rho$ in much the same way as the number of excitations was constrained at the end of Sec. II. This possibility has been studied. It is in fact possible to incorporate such a constraint in the statistical-mechanical formalism, but the structure of the resulting theory is not acceptable. It is certain that this is not a valid procedure. The reason is connected with the fact that ρ_n is not a microscopic variable defined quantum mechanically, but it is only a statistical-mechanical variable. This distinguishes it in an important qualitative way from a variable such as the number of excitations. For at least some physically allowed states of the system, $\rho_s<0$. An interesting sidelight of this observation is that it raises a serious question about the validity of the phenomenological order-parameter theory of Ginsburg and Pitaevskii.[41] That theory rests on a fundamental assumption that $\rho_s\geqslant 0$.

We are driven to consider the statistical-mechanical formulas and the two-fluid equations as valid both above and below T_λ. Experiment shows that when the liquid is slightly disturbed from a state in which it is macroscopically at rest, the motion of the liquid is characteristic of a mixture of two fluids below T_λ and one fluid above T_λ. What is responsible for this change in behavior?

One possibility is that the nature of the solutions of the two-fluid equations changes at T_λ because of the values taken on by the variables entering the equations. To illustrate the point, let us suppose that a small temperature disturbance is generated at some site in the liquid, and that prior to the perturbation, the system is in a homogeneous rest state, i.e., throughout the liquid $v_s=v_n=0$. Now, suppose that the two-fluid equations are valid at all temperatures. The formula for the velocity of second sound in lowest order is[25]

$$C_2=(\rho_s TS^2/\rho_n C_V)^{1/2}. \tag{61}$$

Below T_λ, the formula yields a real number for C_2; but above T_λ, $\rho_s \equiv \rho - \rho_n < 0$, and C_2 is purely imaginary. Therefore, second sound would propagate as a decaying exponential above the λ point, and would lose its identity as a wave motion. Obviously, this argument is incomplete, but it suggests that some light might be shed on the problem considered here by working out the implications of the two-fluid equations above T_λ, even in the approximation in which the ordinary dissipative coefficients are neglected.

In an effort to find a more general explanation for why the flow properties of the liquid change, let us consider a thermodynamic argument. Suppose that $\vec{v}_s$ were treated as a thermodynamic variable. The extensive variable conjugate to $\vec{v}_s$, call it $\vec{Q}$, can be evaluated with the aid of Eq. (16) or (53). If one computes $\partial W/\partial \vec{v}_s = -\vec{Q}$, the result is

$$\vec{Q}=M_s(\vec{v}_n-\vec{v}_s). \tag{62}$$

The internal energy, call it U, would be related to the thermodynamic potential E' considered in Sec. II by

$$U=E'+\vec{Q}\cdot\vec{v}_s. \tag{63a}$$

The differential form is

$$dU=-p\,dV+T\,dS+\vec{v}_n\cdot d\vec{P}'+\mu\,dN+\vec{v}_s\cdot d\vec{Q}. \tag{63b}$$

Recall that in Sec. II, E' was regarded as the internal energy subject to the assumption that $\vec{v}_s$ be a mechanical variable. Now we are dispensing with this last assumption. Next, let us define a Legendre transform of W, call it Y, in the following way:

$$Y(V,T,N,\vec{v}_n,\vec{Q})=W+\vec{Q}\cdot\vec{v}_s. \tag{64a}$$

Then, using Eq. (17), one finds

$$dY=-p\,dV-S\,dT-\vec{P}'\cdot d\vec{v}_n+\mu\,dN+\vec{v}_s\cdot d\vec{Q}. \tag{64b}$$

From the general theory of the stability of thermodynamic systems,[39] it is known that if a diagonal second-order derivative of the type

$$\frac{\partial^2 Y}{\partial Q_i\,\partial Q_i}=\frac{\partial v_{si}}{\partial Q_i}=\left(\frac{\partial Q_i}{\partial v_{si}}\right)^{-1} \tag{65}$$

is negative, the system will be unstable. In Eq. (65), the subscript i refers to the ith Cartesian component of a vector. This criterion is closely related to one discussed by Hohenberg and Martin in Ref. 35. However, it seems that there is an error in their work, because Eqs. (3.45) and (3.8) are inconsistent with each other. The error is not trivial, because instead of their free energy W/β, one must use a Legendre transform with respect to $\vec{v}_s$ to get the right-hand side of Eq. (3.45). Nevertheless, the *idea* which they propose is suggestive, and is the subject which we shall examine here.

First, let us evaluate the derivatives in Eq. (65) under the conditions that $v_s=v_n=0$, and let the superscript zero denote these system points. Then one finds

$$\left(\frac{\partial^2 Y}{\partial Q_i\,\partial Q_i}\right)^0=-\frac{1}{M_s^0}. \tag{66}$$

But we also have

$$M_s^0\begin{cases}>0 & \text{for } T<T_\lambda\\ =0 & \text{for } T=T_\lambda\\ <0 & \text{for } T>T_\lambda\,.\end{cases} \tag{67}$$

Therefore, under the assumption that $\vec{v}_s$ is a thermodynamic variable, the system at rest would be *unstable* for $T<T_\lambda$. To determine whether the system at rest would actually be stable for $T>T_\lambda$ requires further calculation, but at least the relations in (67) would be consistent with that possibility. The element of uncertainty above T_λ is connected with the possibility that the state of the system corresponds to a saddle point of the internal energy function in the space of the independent thermodynamic variables. Note that as T approaches T_λ, the *reciprocal* of $\partial v_{si}/\partial Q_i$ approaches zero, and not $\partial v_{si}/\partial Q_i$ itself, as one might surmise from Eq. (3.45) in Ref. 35. These results suggest that characteristic two-fluid behavior may be associated with *instability* of the liquid with respect to small fluctuations in $\vec{Q}$. The change in the sign of the superfluid mass here is the signal for the change in the character of the liquid, just as it was in the illustration involving the velocity of second sound. One can use the data in Fig. 1 to evaluate the derivative in Eq. (65) numerically for all values of $|\vec{v}_s-\vec{v}_n|$ and for any temperature, and we shall do this in part in the case where there are no direct interactions among the excitations. Recall that in this approximation $T_\lambda=2.415$ °K. For illustrative purposes, let us suppose $v_n=0$ and that only the $i=1$ Cartesian component of $\vec{v}_s$ is nonzero. Then one finds that at $T=2.20$ °K, $(\partial Q_1/\partial v_{s1})_{\vec{v}_n=0}=0$ near $v_s=15$ m sec^{-1}, and that it is negative for smaller velocities and positive for higher. At $T=2.40$ °K, just 0.015 °K below T_λ, $(\partial Q_1/\partial v_{s1})_{\vec{v}_n=0}$ vanishes near $v_s=5$ m sec^{-1}. By making a Taylor-series expansion of $F(v_s)$ in powers of v_s [the desired result can be found by taking $\gamma=0.0$ in Eqs. (126)–(129) in Sec. IV], one can show that the threshold velocity for stability varies as $(T_\lambda-T)^{1/2}$ when T approaches

T_λ from below. For $T > T_\lambda$ and $v_n = 0$, $\partial Q_1/\partial v_{s1} > 0$ for all values of v_s. In summary, one finds that for $T < T_\lambda$ and $v_n = 0$, there is some range of velocities contiguous with $v_s = 0$ for which the system would be *unstable* with respect to fluctuations in the components of $\vec{Q}$; whereas for $T > T_\lambda$ and $v_n = 0$ the system might be stable in this respect for all values of $\vec{v}_s$.

In the foregoing discussion, the velocity and temperature ranges for stability and instability of the liquid are almost exactly reversed from those described by Feynman.[40] So let us consider an alternative way of dealing with the microscopic theory that would lead us to the same conclusions regarding the stability of the system that Feynman reached. The essential observation here is that an *extensive* variable $\vec{P}_0$ may be introduced into the theory by the definition

$$\vec{P}_0 \equiv Nm\vec{v}_s\,. \tag{68}$$

Then $\vec{v}_s$ is not a thermodynamic variable itself, but is just a convenient shorthand notation for $\vec{P}_0/Nm$, and must be dealt with in that way in the quantum-mechanical and statistical-mechanical formulas in Sec. II. The proper form of Eq. (9) for the energy eigenvalues would then be

$$E' = E_0 + \frac{P_0^2}{2Nm} + \frac{1}{Nm}\vec{P}_0\cdot\sum n_i\vec{p}_i + \sum n_i\epsilon_i\,. \tag{69}$$

The free energy W of Eq. (16) should be written

$$W(\vec{P}_0, \vec{v}_n) = E_0 + \frac{P_0^2}{2Nm} - \vec{P}_0\cdot\vec{v}_n - kT\sum\ln(1+n_i)\,, \tag{70}$$

where the n_i are given by Eq. (13) when Eq. (68) is taken into account. From Eq. (70), one finds that the variable conjugate to $\vec{P}_0$, let us call it $\vec{u}$, is

$$\begin{aligned}\vec{u} &= \frac{\partial W}{\partial\vec{P}_0}\\ &= \frac{\rho_s}{\rho}(\vec{v}_s - \vec{v}_n)\,.\end{aligned} \tag{71}$$

When the thermal equilibrium values of n_i are used to evaluate E', given by Eq. (69), the resulting expression represents the internal energy, for

$$E' = E'(V, S, \vec{P}', N, \vec{P}_0)$$

is a fundamental relation expressed completely in terms of extensive variables of the system; the differential of the internal energy is

$$dE' = -p\,dV + T\,dS + \vec{v}_n\cdot d\vec{P}' + \mu\,dN + \vec{u}\cdot d\vec{P}_0\,. \tag{72}$$

It appears that this approach is just as satisfactory as the one where $\vec{v}_s$ itself was treated as a thermodynamic variable. In fact, it seems to lead to the same results as were obtained in Sec. II and earlier in this section, with two exceptions, which we shall illustrate by considering the case of noninteracting excitations. Instead of Eq. (34b), one now finds that the chemical potential satisfies

$$\begin{aligned}\mu &= \left(\frac{\partial W}{\partial N}\right)_{T,V,\vec{v}_n,\vec{P}_0}\\ &= m\left(e_0 + \rho\frac{\partial e_0}{\partial\rho} + \frac{1}{V}\sum n_i\frac{\partial\epsilon_i}{\partial\rho}\right.\\ &\qquad\left. - \frac{1}{2}v_s^2 + \frac{\rho_n}{\rho}v_s^2 - \frac{\rho_n}{\rho}\vec{v}_n\cdot\vec{v}_s\right).\end{aligned} \tag{73}$$

The pressure as well as other quantities calculated as first partial derivatives of W while N is held constant are the same as before. The analog of Eq. (34f) is

$$z - \frac{\mu}{m} = \frac{1}{2}v_s^2 + \frac{\rho_n}{\rho}\vec{v}_n\cdot\vec{v}_s - \frac{\rho_n}{\rho}v_s^2\,. \tag{74}$$

It is easy to see that this same result holds when interactions among the excitations are present. The second exception is in the stability properties of the system. The general theory of stability[39] now indicates that one should examine the diagonal second-order derivatives of the type

$$\frac{\partial^2 W}{\partial P_{0i}\,\partial P_{0i}} = \frac{\partial u_i}{\partial P_{0i}}\,. \tag{75}$$

At $v_n = P_0 = 0$, this yields

$$\left(\frac{\partial^2 W}{\partial P_{0i}\,\partial P_{0i}}\right)^0 = \frac{M_s^0}{M^2}\,. \tag{76}$$

Now, one reaches the opposite conclusions regarding the stability of the homogeneous system at rest from those deduced from Eq. (66). It is clear, in fact, that the stability properties inferred from Eqs. (71) and (75) for $v_n = 0$ and all values of P_0 would be compatible with those described by Feynman. Those results can be understood easily with the aid of Fig. 5, provided that the abscissa be interpreted in accordance with Eq. (68).

The theory based on the variable $\vec{P}_0$ seems to be just as capable of accounting for the change of flow properties at T_λ in terms of a change in stability as the theory based on the variable $\vec{v}_s$. Which is more appropriate in treating liquid ^{4}He is still not known. A study which provides a qualitative analysis of the detailed mechanism by which thermodynamic stability affects flow properties is needed to solve that problem, and the answer cannot be given now.

Usually a system does not attain a state of equilibrium that is unstable according to ordinary thermodynamic criteria because fluctuations are not counteracted by a restoring force then. However, factors which have not been mentioned so far may permit exceptional behavior of liquid ^{4}He in this regard. For example, because the circulation of $\vec{v}_s$ is quantized, fluctuations of $\vec{P}_0$ involving exchanges between neighboring regions might be inhibited by the necessity to supply simultaneously the energy of a vortex core, at least in a simply connected region. On the other hand, viscosity as well as vortex-core requirements are factors that might suppress fluctuations in $\vec{Q}$, and consequently suppress the usual effects of thermodynamic instability.

It was demonstrated in Sec. II that interactions among elementary excitations present no obstacle in the theoretical formalism, at least if they are in the class discussed there. It is conceivable that they are essential in understanding the behavior of the liquid, particularly near the temperature where the superfluid transition occurs. Therefore we shall now investigate effects of some simple interactions.

The central problem here is to find explicit self-consistent solutions of Eq. (51), which determines the occupation numbers, and then to use them in evaluating thermodynamic functions. First we must deal with the question of how the coefficients f_{ij}, f_{ijk}, etc., are to be determined. In principle, they could be calculated, at least approximately, by using the CBF formalism. However, definitive results would require treatment of high-excited states with an accuracy that has not yet been achieved by that method. That approach may be the most reliable when CBF theory is developed further, but it cannot solve our problem at this time. An alternative approach is to follow the lead of Bendt, Cowan, and Yarnell,[29] who extracted average values of f_{ij} from neutron-scattering data with the aid of certain simplifying assumptions. One of their implicit assumptions is that the liquid is always homogeneous and stationary. We shall see in Sec. IV that there are reasons to believe that these conditions do not exist in the liquid near T_λ, but that quantized vortices are present there. If vortices were present, there would be a mantle of high roton density near each core. If such mantles were present but one neglected them in extracting values of f_{ij} from neutron-scattering data, large errors would be made. Therefore, we shall proceed in a different manner, and we shall set a rather modest goal for our analysis, viz., to see effects of interactions among excitations on observable properties of the liquid somewhat qualitatively. For simplicity, we shall limit the discussion to pair interactions, corresponding to terms in the energy eigenvalues of the form $(1/2N)\sum f_{ij}n_i n_j$. There are two choices of f_{ij} that have been studied in similar contexts in the literature.[1,42-44] At first we shall deal with them separately, and later we shall discuss the situation when they are present simultaneously.

The first case that we shall consider has a direct analog in electromagnetic theory, and we shall refer to it as the polarization interaction. It was originally discussed by Feynman on p. 274 of Ref. 1. The plausibility of this model was reinforced by the somewhat later work of Feynman and Cohen,[6] who found that a dipolar velocity field, the so-called backflow, was associated with a roton; this suggests that rotons interact as if they were dipoles and consequently influence each other through a polarization interaction. From the continuity equation, which is implied by the Schrödinger equation for the many-body system, one infers that when the liquid is in an energy eigenstate, then

$$\vec{\nabla}\cdot\vec{j}(\vec{r})=0\,. \tag{77}$$

Here $\vec{j}(\vec{r})$ is the quantum-mechanical mass-current density. When the density ρ and flow velocity $\vec{v}_s$ are uniform throughout the system, $\vec{j}(\vec{r})$ is independent of spatial position, and is given by

$$\vec{j}(\vec{r})=\frac{\vec{P}}{V}=\rho\vec{v}_s+\frac{1}{V}\sum n_i\vec{p}_i\,. \tag{78}$$

Feynman noted the mathematical parallel between Eqs. (77) and (78) and the equations for electrical phenomena when the free charge density is zero:

$$\vec{\nabla}\cdot\vec{D}=0 \tag{79}$$

and

$$\vec{D}=\vec{E}+4\pi\vec{\mathcal{P}}\,. \tag{80}$$

Here $\vec{D}$ is the electrical displacement, $\vec{E}$ is the macroscopic electric field, and $\vec{\mathcal{P}}$ is the polarization. In the electrical case, it is known from a type of analysis originally due to Lorentz that if the polarization is due to dipoles that are located at random positions in space, then the *local* electric field $\vec{E}_l$ experienced by a typical dipole is related to quantities appearing in (80) by

$$\vec{E}_l=\vec{E}+\tfrac{4}{3}\pi\vec{\mathcal{P}}\,. \tag{81}$$

Feynman suggested that in the case of the ^{4}He liquid, the local velocity $\vec{w}$ experienced by an excitation would be made up of two parts, viz., the average superfluid velocity $\vec{v}_s$, analogous to the macroscopic electric field $\vec{E}$, and a part due solely to the dipolar field associated with other excitations, $(1/\rho V)\sum n_i\vec{p}_i$. Then the analog of Eq. (81) would be

$$\vec{w}=\vec{v}_s+\frac{\alpha}{\rho V}\sum n_i\vec{p}_i\,, \tag{82}$$

where $\alpha=\frac{1}{3}$ in the Lorentz-type analysis. Feynman said that the excitation energy which determines the occupation number n_i should involve $\vec{p}_i \cdot \vec{w}$ instead of just $\vec{p}_i \cdot \vec{v}_s$. This would be a natural consequence of the microcanonical formalism if we took

$$\frac{1}{2N}\sum f_{ij}n_i n_j = \frac{1}{2N}\frac{\alpha}{m}\left(\sum n_i \vec{p}_i\right)^2 \qquad (83)$$

in the expression for the energy eigenvalues, given in Eq. (8b). Then imposing the condition that W in Eq. (14) be stationary with respect to variations in the occupation numbers, one finds the following special case of Eq. (51):

$$n_i = \frac{1}{\exp\{\beta[\epsilon_i + \vec{p}_i \cdot (\vec{w} - \vec{v}_n)]\} - 1}, \qquad (84)$$

where $\vec{w}$ is given by (82). When the self-consistent values of n_i, i.e., the solutions of (82) and (84), are used to evaluate $\vec{w}$, one can express Eq. (84) in the following simple form with the aid of Eq. (22):

$$n_i = \frac{1}{\exp\{\beta[\epsilon_i + \vec{p}_i \cdot (\vec{v}_s - \vec{v}_n)(1 - \alpha\rho_n/\rho)]\} - 1}. \qquad (85)$$

The thermodynamic potential W then can be written

$$W = E_0 + \tfrac{1}{2}Nm v_s^2 - N_m \vec{v}_s \cdot \vec{v}_n - kT\sum \ln(1 + n_i) - \frac{1}{2N}\frac{\alpha}{m}\left(\sum n_i \vec{p}_i\right)^2, \qquad (86a)$$

and the internal energy is

$$E = E_0 + \tfrac{1}{2}Nm v_s^2 + \vec{v}_s \cdot \sum n_i \vec{p}_i + \sum n_i \epsilon_i + \frac{1}{2N}\frac{\alpha}{m}\left(\sum n_i \vec{p}_i\right)^2. \qquad (86b)$$

Feynman noted that a polarization interaction of this type, with $\alpha = \frac{1}{3}$, would raise the temperature T_λ above that for a noninteracting system. It is straightforward to verify this by making a Taylor-series expansion of $\vec{P}$ in powers of $\vec{v}_s$. Of course, his analysis was carried out before neutron-scattering data were available for the dispersion curve; therefore, it was not obvious that this type of interaction, acting alone, would increase the discrepancy between calculated and experimental values of T_λ by an appreciable amount. This effect could possibly be offset by other interactions not yet considered. However, there also seems to be a problem at a more fundamental level with part of Feynman's argument based on analogy with electrostatics. The point in question is whether it is reasonable to suppose that $\vec{v}_s$ corresponds to $\vec{E}$, the *macroscopic* electric field, as Feynman did. In electrostatics, that field is in general partly due to sources external to the dielectric, but it is partly due to aligned dipoles in the dielectric itself. Now in the liquid case, as the theory is formulated here, and as it seems to be in Feynman's treatment, it is assumed that $\vec{v}_s$ is fixed independently of the elementary excitation states. Or, said another way, for the dipole model, $\vec{v}_s$ does not depend on the state of polarization. Since this is true at the quantum-mechanical level, i.e., for the energy eigenvalues, it is also true in the statistical-mechanical formulas. Clearly, this is not consistent with $\vec{v}_s$ being treated as the analog of the macroscopic electric field. Therefore, a reexamination of the analogy with electrostatics is called for, and we shall deal with that next.

Let us consider a thought experiment as schematized in Fig. 6. The pistons D and E move with a common velocity $\vec{v}_s$ and force superfluid to flow through the region A that is bounded at its ends by superleaks B and C, which are assumed to be perfect thermal insulators. The length X of the region A is much less than the radius of the tube F. The liquid in region A is the system of interest. The remainder of the apparatus just provides a method for fixing the velocity $\vec{v}_s$ in A while it is otherwise isolated as far as energy transfer is concerned. In our idealization, we shall suppose that the density is constant throughout the liquid. Now suppose that excitations, modeled as dipoles, appear in region A, but nowhere else, while $\vec{v}_s$ remains constant. Then a Lorentz-type calculation of the *local* velocity field due to the dipoles alone is mathematically equivalent to that for the dipole contribution to the local electric field in a dielectric slab. When the *external field* $\vec{v}_s$ is added in, one finds that the local field experienced by any dipole is

$$\vec{w} = \vec{v}_s - \frac{2}{3\rho V}\sum n_i \vec{p}_i. \qquad (87)$$

This leads to the conclusion that one should take $\alpha = -\frac{2}{3}$ in Eq. (82) and the succeeding equations. On the other hand, for rotons aligned parallel to the large flat faces in a thin liquid sample, one finds $\alpha = \frac{1}{3}$, the same value that Feynman used.

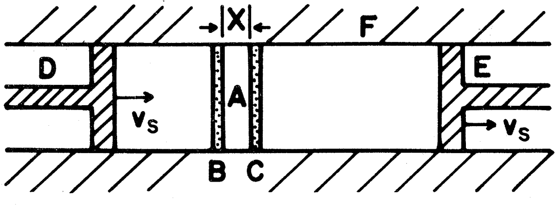

FIG. 6. Schematic diagram of apparatus for a thought experiment for analyzing the polarization interaction among rotons. See text for details.

In general the value of α depends on the shape of the sample because of "depolarization" contributions to the velocity, which can be associated with surface terms. A backflow field of either electric or magnetic dipole type aligned with the axis in a long narrow region also gives $\alpha = \frac{1}{3}$. It may be noteworthy that for $\alpha = -\frac{2}{3}$, the calculated transition temperature T_λ is 2.15 °K at zero pressure, and 1.90 °K at 25.3 atm. The corresponding experimental values are 2.17 and 1.82 °K, respectively. The zero-pressure calculation was based on the density and dispersion curve described earlier. The high-pressure calculation was based on the density $N/V = 0.0259$ atom Å^{-3}, and on the neutron-scattering data of Henshaw and Woods[45] for the dispersion curve at 1.1 °K. Despite this remarkable agreement between calculated and experimental values of T_λ as a function of pressure, it is clear that the polarization interaction alone cannot account for other details of the behavior of liquid ^{4}He. This can be made evident by the following considerations. Suppose the liquid is contained in a simply connected region bounded by stationary walls, and that the system remains homogeneous. Then $v_s = v_n = 0$, and the only solution of Eqs. (82) and (84) consistent with Eq. (22) occurs when $\vec{w} = 0$. Then the polarization interaction acting alone would not produce a reduction in the effective roton energy gap as the temperature increases toward T_λ. On the other hand, neutron-scattering experiments show that the gap decreases.[29,33] Furthermore, the occupation numbers for the excitations would not be affected by the polarization interaction under these circumstances, and consequently the entropy would not be affected by it either. It is straightforward to show that the four forms of the specific heat at constant volume still satisfy the formula for noninteracting excitations given by Eq. (58) when $v_s = v_n = w = 0$. Therefore the polarization interaction acting alone cannot produce the logarithmic singularity in the specific heat. One may question the validity of our treatment on the grounds that all of the excitations were regarded as being associated with dipoles, whereas the calculation of Feynman and Cohen just indicates that this is true for rotons, and says nothing about the situation for phonons. There is, in fact, no reason to expect that a dipolar backflow will be appreciable for phonons. It is therefore important to note that above about 1.1 °K, less than 4% of the contribution to the normal fluid density is due to phonons; and so in the temperature range where interactions might be important for thermodynamics, little error is introduced by treating all of the excitations as if they were dipoles. If, as a matter of principle, one wished to exclude the phonons from the polarization interaction, the general theory could easily be adapted to that case. The qualitative conclusions reached regarding T_λ, the roton energy gap, and the entropy would remain the same.

Next, let us consider the second case, the mean-field interaction, which involves a single dimensionless coupling constant that we shall represent by γ. The pair contribution to the energy eigenvalues in this model may be represented as follows:

$$\frac{1}{2N}\sum f_{ij} n_i n_j = -\frac{N\gamma\epsilon_0}{2}\left(\frac{1}{N}\sum{}' n_i\right)^2$$
$$= -\tfrac{1}{2}N\gamma\epsilon_0 f^2 . \qquad (88)$$

The quantity ϵ_0 appearing in Eq. (88) is the minimum roton gap energy for low excited states. Neutron-scattering data[29,33] on the temperature dependence of the roton gap energy indicates that γ should be chosen positive. The prime on the sum in the second term means that it is restricted to a subset of the excitations, which we shall take, somewhat arbitrarily, to be those having energy greater than or equal to ϵ_0 in our example, and we shall refer to those excitations as rotons. If all excitations, including phonons, were included in the sum, then some of the energy eigenvalues would be less than E_0, the assumed ground-state energy, and the model would be unsatisfactory from the standpoint of logic. What is perhaps less obvious is that there must be an upper limit, call it $\mathfrak{N}$, on the number of excitations in the restricted sum, for otherwise there would be multiexcitation states having energy less than E_0. The quantity f is just the ratio of the number of rotons to the total number of particles in the system. For this form of the pair interaction, the occupation numbers for the *rotons* are determined by the following formulas when the system is in themodynamic equilibrium:

$$n_i = \frac{1}{\exp\{\beta[\epsilon_i + \vec{p}_i \cdot (\vec{v}_s - \vec{v}_n) - \gamma\epsilon_0 f]\} - 1} \qquad (89a)$$

and

$$f = \frac{1}{N}\sum{}' n_i . \qquad (89b)$$

The *phonon* occupation numbers are the same as in the noninteracting case. When the n_i are solutions of these equations, the thermodynamic potential W is

$$W = E_0 + \frac{1}{2}Nmv_s^2 - Nm\vec{v}_s \cdot \vec{v}_n - kT\sum \ln(1+n\ )$$
$$+ \frac{1}{2}N\gamma\epsilon_0\left(\frac{1}{N}\sum{}' n_i\right)^2 , \qquad (90)$$

and the internal energy is

$$E = E_0 + \frac{1}{2} N m v_s^2 + \vec{v}_s \cdot \sum n_i \vec{p}_i + \sum n_i \epsilon_i - \frac{1}{2} N \gamma \epsilon_0 \left(\frac{1}{N} \sum{}' n_i \right)^2 . \tag{91}$$

To illustrate the effect of the mean-field interaction, let us take $\gamma = 0.2$. This value of γ is appreciably smaller than that which one would find by using the pair interaction formula given by Bendt and co-workers.[29] For $\gamma = 0.2$, it turns out that there are solutions of Eq. (89) for a range of temperatures $0 < T \lesssim 3.6$ °K, and there are *no* solutions when $T \gtrsim 3.6$ °K. Furthermore, for any temperature $T \lesssim 3.6$ °K and for any velocity $\vec{V} = \vec{v}_n - \vec{v}_s$ in the range from $V = 0$ up to some maximum value which depends on the temperature, there are *two* solutions of Eqs. (89a) and (89b). The solution of those equations were first sought by an iteration procedure. When it was found that the results did not converge for large values of V or T, a study was made of the conditions for the threshold above which solutions no longer exist. This was done, for fixed values of V and T, by computing the right-hand side of Eq. (89b) as a function of f, and noting the value where (89b) was satisfied. Representative plots of the two sides of Eq. (89b), for $T = 2.0$ °K and three different values of V near the threshold at that temperature, are shown in Fig. 7. The threshold velocity U, below which there are always solutions of Eq. (89) and above which there are none is shown as a function of temperature in Fig. 8. For a homogeneous system in which $\vec{V}$ is the same everywhere, the occupation numbers will contain a chemical potential for rotons when T and V are such that no solution of Eq. (89) exists. In fact, if a solution of Eq. (89) does occur at a given T and V, but the calculated value of the total number of rotons exceeds the upper limit $\mathfrak{N}$, mentioned earlier, then a chemical potential for rotons also must occur in the occupation numbers. If the system does not remain homogeneous, there is another way of dealing with the conditions at large velocities, that does not involve a chemical potential for rotons. That case is discussed in Sec. IV, where the density of the liquid is assumed to undergo a rapid variation in the high-velocity region, and vortex cores are thereby formed.

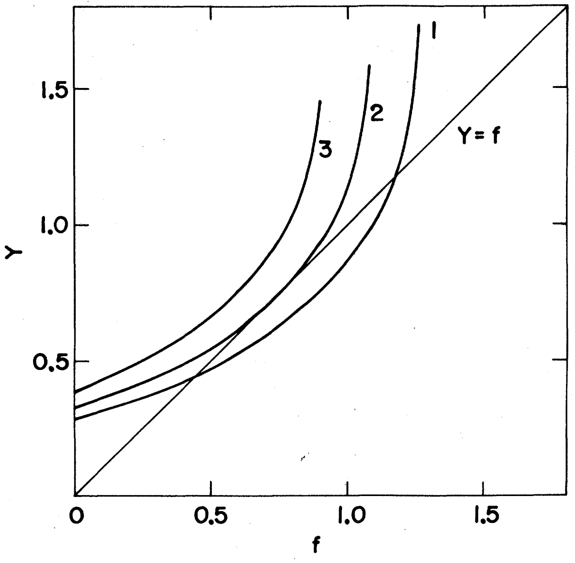

FIG. 7. Right-hand side of Eq. (89b), represented by Y, as a function of f, where n_i is given by Eq. (89a). All curves are for conditions near threshold at $T = 2.0$ °K. For $V = |\vec{v}_n - \vec{v}_s|$, they correspond to the following velocities: curve 1, $V = 44.0$ m/sec; curve 2, $V = 46.0$ m/sec; curve 3, $V = 48.0$ m/sec. Solutions to Eq. (89b) occur at the intersections of the curves with the straight line $Y = f$. A mean-field interaction is assumed, with $\gamma = 0.2$.

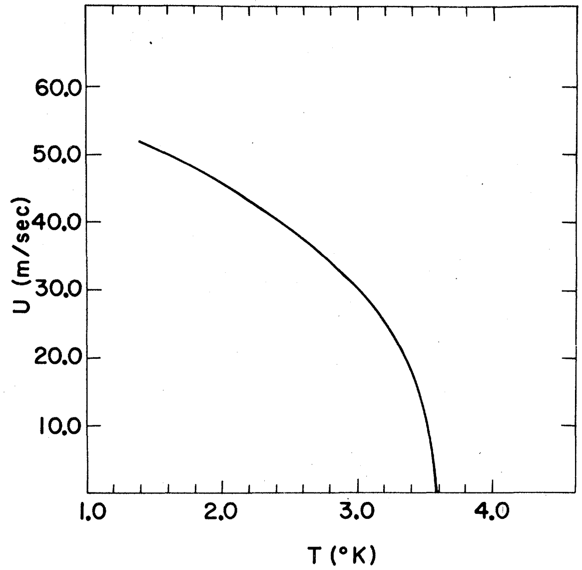

FIG. 8. Threshold velocity U, for solutions to Eqs. (89a) and (89b), as a function of temperature. A mean-field interaction is assumed, with $\gamma = 0.2$.

Evaluation of W at $v_n = 0$ gives the Helmholtz potential

$$F(v_s) = E_0 + \frac{1}{2} N m v_s^2 - kT \sum \ln(1 + n_i) + \frac{1}{2} N \gamma \epsilon_0 \left(\frac{1}{N} \sum{}' n_i \right)^2 . \tag{92}$$

Under the assumption that the chemical potential for rotons is zero for $v_s < U$, the isotherms of $F(v_s)$ are shown in Fig. 9 for $\gamma = 0.2$. They are qualitatively the same as for the noninteracting case, shown in Fig. 5, except for the fact that they terminate at $v_s = U$ rather than at the Landau critical velocity. The solution of Eq. (89) corresponding

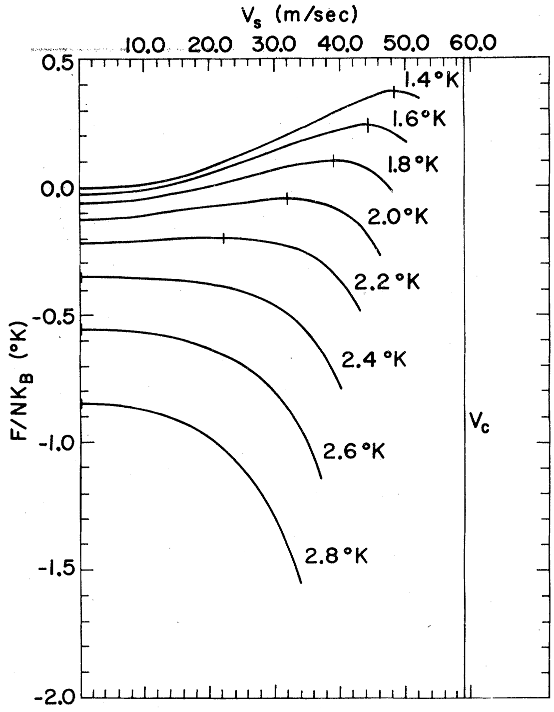

FIG. 9. Free energy per particle as a function of superfluid velocity v_s when $v_n = 0$. Each curve is an isotherm. The calculated free energy is based on Eq. (92) with $\gamma = 0.2$, but E_0 has been subtracted out of the formula. The vertical lines mark the maxima on the isotherms. V_c is the Landau critical velocity. The isotherms terminate at $v_s = U$, where U is given in Fig. 8.

to the smaller of the two values of f at each value of T and v_s was used in the evaluation of the free energy. This choice was based on the idea that the physical solution should tend continuously to that of the noninteracting system as γ tends to zero, and it is consistent with the results of a computer evaluation of the free energy for *both* solutions at $T = 2.0$ °K with $v_s = 44.0$ m sec^{-1}. The transition temperature T_λ is shifted downward by the interaction to about 2.365 °K from 2.415 °K. All four forms of the specific heat at constant volume, evaluated at $\vec{v}_s = \vec{v}_n = 0$, again have the same value, and vary smoothly from $T = 0$ to the threshold temperature, $T_t = 3.6$ °K, as indicated in Fig. 4. The entropy is also shown there.

Figure 4 is useful in studying possible phase transitions in the stationary, homogeneous liquid. If the number of excitations reaches the constraining limit $\mathfrak{N}$ at a temperature T_n such that $T_n < T_t$, the liquid will undergo a second-order phase transition there. One can understand why this is so in the following way. The roton chemical potential will be zero below T_n, and will tend to zero as the temperature approaches T_n from above. Hence, the occupation numbers, and in turn the entropy, will be continuous at T_n. The partial derivative of the roton chemical potential will not be zero at T_{n+}, however, and that is what produces the anomaly in the specific heat. On the other hand, if as temperature increases, the threshold T_t is reached before T_n, then the system will undergo a first-order transition at T_t. Again, the roton chemical potential will be zero for $T < T_t$, but it will jump to some finite value at T_{t+}, so that the constraint on $\sum' n_i/N$ will be satisfied as an equality there, and that is what produces the discontinuity in the occupation numbers and in the entropy as T passes through T_t. In this case, the specific heat C_V diverges as T approaches T_t from below, $C_V \sim (T_t - T)^{-1/2}$ for $T \to T_{t-}$, but the transition is still first order because of the discontinuity in the entropy at T_t. The stated temperature dependence of C_V is derived later in this discussion. If T_n and T_t should happen to coincide, a second-order transition would occur. Even though it would seem to require a spectacular accident in nature for $T_n = T_t = T_\lambda$, this case still merits close examination to determine whether it might account for the logarithmic divergence in the specific heat observed in liquid ^{4}He. A detailed analysis is given below.

First, let us note that in Fig. 4, the specific heat appears to be diverging as $T \to T_{t-}$. A qualitative understanding of this behavior can be gained with the aid of Fig. 10, where the right-hand side

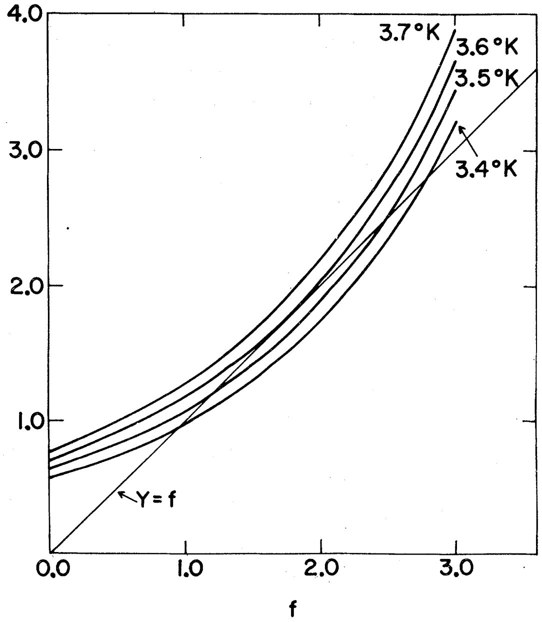

FIG. 10. Right-hand side of Eq. (89b), represented by Y, plotted as a function of f for several different temperatures near T_t, and for $V = |\vec{v}_n - \vec{v}_s| = 0$. Solutions of Eq. (89b) occur at the intersections of the curves with the straight line $Y = f$.

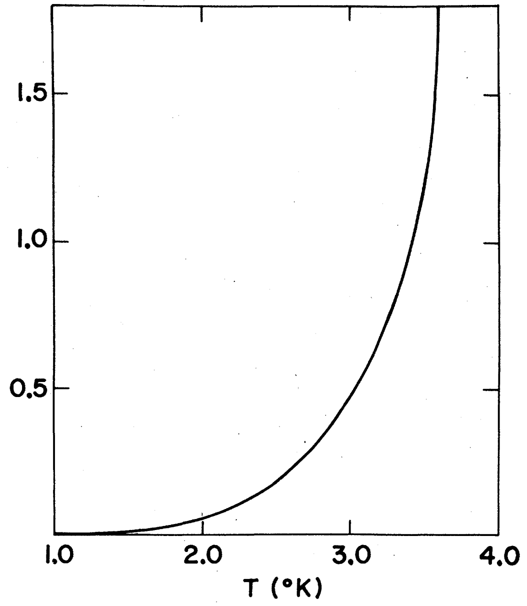

FIG. 11. Plot of f, corresponding to the physical solutions of Eq. (89b), as a function of temperature when $V = |\vec{v}_n - \vec{v}_s| = 0$.

of Eq. (89b) is plotted as a function of f for severa values of temperature, and for $V = |\vec{v}_s - \vec{v}_n| = 0$. Solutions to Eq. (89b) occur at the intersection of the curves with the diagonal line $Y = f$; and, as noted earlier, we shall suppose that the smaller values of f give the physical solutions, which are plotted as a function of temperature in Fig. 11. In that figure, one can see that df/dT appears to be diverging as $T \to T_{t-}$. We shall see shortly that this behavior of df/dT induces a singularity in C_V. To work out the mathematical description of these phenomena, let us start by representing the right-hand side of Eq. (89b) as

$$Y(f) = \frac{1}{N} \sum{}' n_i , \qquad (93)$$

where

$$n_i = 1/(e^{\beta(\epsilon_i - \gamma\epsilon_0 f)} - 1) . \qquad (94)$$

Let f_0 represent the solution of $Y = f$ at T_t. Then, for f near f_0 and T near T_t, we shall make a double Taylor-series expansion of Y and keep only terms through second order; this gives

$$\begin{aligned} Y = f_0 &+ \left(\frac{\partial Y}{\partial T}\right)_0 (T - T_t) + \left(\frac{\partial Y}{\partial T}\right)_0 (f - f_0) \\ &+ \frac{1}{2}\left[\left(\frac{\partial^2 Y}{\partial T^2}\right)_0 (T - T_t)^2 + 2\left(\frac{\partial^2 Y}{\partial T \partial f}\right)_0 (T - T_t) \right. \\ &\left. \times (f - f_0) + \left(\frac{\partial^2 Y}{\partial f^2}\right)_0 (f - f_0)^2\right] . \end{aligned} \qquad (95)$$

Note from Fig. 9 that $(\partial Y/\partial T)_0 = 1$. For any T near T_t, we can solve the equation

$$Y = f , \qquad (96)$$

which is equivalent to Eq. (89b), by using Eq. (95). To express the equations in a more compact form, let us introduce the following notation:

$$a = \frac{1}{2}\left(\frac{\partial^2 Y}{\partial f^2}\right)_0 , \quad b = \left(\frac{\partial^2 Y}{\partial T \partial f}\right)_0 , \quad c = \left(\frac{\partial Y}{\partial T}\right)_0 ,$$
$$d = \frac{1}{2}\left(\frac{\partial^2 Y}{\partial T^2}\right)_0 , \quad t = T_t - T , \quad F = f - f_0 . \qquad (97)$$

Then Eqs. (96) and (97) give

$$aF^2 - bFt - ct + dt^2 = 0 , \qquad (98)$$

which is a quadratic equation in the variable F. The physical solution, i.e., the one for which f is the smallest, is given by

$$\begin{aligned} f(T) = f_0 + (1/2a)\{b(T_t - T) - [4ac(T_t - T) + (b^2 - 4ad) \\ \times (T_t - T)^2]^{1/2}\} , \end{aligned} \qquad (99)$$

where the relations in (97) have been used again. From Eq. (99) it follows that

$$\frac{df}{dT} = \frac{1}{2a}\left(-b - \frac{\frac{1}{2}[-4ac - 2(b^2 - 4ad)(T_t - T)]}{[4ac(T_t - T) + (b^2 - 4ad)(T_t - T)^2]^{1/2}}\right) \qquad (100)$$

For T just slightly less than T_t, this reduces to

$$\frac{df}{dT} = \frac{1}{2a}\left[-b + \tfrac{1}{2}\left(\frac{4ac}{T_t - T}\right)^{1/2}\right] . \qquad (101)$$

The entropy is given by Eq. (10), and we shall write it as

$$S = S_{\mathrm{phon}} + S_{\mathrm{rot}} . \qquad (102)$$

The phonon part will vary smoothly as T passes through T_t, and so we shall focus on the roton part. Then

$$\begin{aligned} C_{V\,\mathrm{rot}} &= T\left(\frac{\partial S_{\mathrm{rot}}}{\partial T}\right)_V \\ &= k \sum{}' \left[\left(\ln \frac{1 + n_i}{n_i}\right) \frac{\partial n_i}{\partial T}\right] \\ &= \sum{}' (\epsilon_i - \gamma\epsilon_0 f) \frac{\partial n_i}{\partial T} \\ &= \sum{}' \left[-n_i(n_i + 1)(\epsilon_i - \gamma\epsilon_0 f) \right. \\ &\quad \left. \times \left(-\frac{1}{kT^2}(\epsilon_i - \gamma\epsilon_0 f) - \frac{\gamma\epsilon_0}{kT}\frac{df}{dT}\right)\right] . \end{aligned} \qquad (103)$$

The term involving df/dT induces the behavior

$C_V \sim (T_t - T)^{-1/2}$. This temperature dependence of C_V is in agreement with the result found by Jäckle,[42] who used Boltzmann statistics in treating the rotons.

Provided that the liquid remains stationary and homogeneous, the behavior of the entropy and specific heat at constant volume would be the same in the presence of both the polarization and mean-field interaction as that which occurs when only the latter interaction is present. This is a consequence of the fact that the polarization interaction does not affect the occupation numbers at $v_s = v_n = 0$. However, the temperature T_λ would be determined in part by the polarization interaction. From the foregoing analysis one can conclude that if the liquid remains homogeneous, then no combination of these two interactions can produce the logarithmic specific-heat anomaly observed in liquid ^{4}He. Perhaps more important than the quantitative failure of such a theory is the fact that it does not provide a causal link between the condition $\rho_n = \rho$ at $v_s = v_n = 0$, where the flow properties of the liquid change, and a specific-heat anomaly. One can now draw much stronger conclusions regarding a basic inadequacy of these interactions than was done by others who studied them in earlier work.[42,44] For here it is clear that the formalism can deal with these interactions accurately, and there is no reason to question the reliability of the results because of widths associated with the energy of excitations.

Obviously, we cannot rule out the possibility that some other kind of interaction is responsible for the λ transition in liquid ^{4}He under the condition that the liquid remains stationary and homogeneous, and that possibility is certainly worthy of further study. However, there is another approach to a possible solution of this problem, and we shall consider that in Sec. IV.

IV. QUANTIZED VORTICES IN LIQUID ^{4}He

Substantial experimental effort has been invested in probing the structure of quantized vortices in rotating liquid ^{4}He systems for about the last ten years.[46-52] However, theoretical work in this area[2,47,53,54] has not been very extensive, and the picture formed from it is still very incomplete and parts of it still must be regarded as quite tentative. In particular, the structure of the vortex cores and the properties of the roton mantle surrounding it at finite temperatures still represent problems of considerable interest that have not been solved completely. A major incentive for studying such details is derived from the fact that it is widely believed that creation of quantized vortices is the main factor which determines critical velocities in flowing He II, at least under certain circumstances. In that connection, calculation of the nucleation energy for vortices is also a matter of great interest which is not yet completely settled. Part of the work discussed in this section bears on solutions to those problems.

However, the primary motivation for the analysis given here is derived from the following ideas: (i) the thermodynamic potential curves in Figs. 5 and 9 suggest that the state of lowest free energy, particularly for a temperature range beginning somewhat below T_λ, may be one in which the liquid is flowing; and (ii) there is a need to understand how the change in the flow characteristics of the liquid are linked causally with the specific-heat anomaly observed at T_λ. If the free energy of the liquid containing vortices were less than that of the stationary liquid, then vortices should be excited thermally even when the walls of the container are at rest. That possibility together with its connections with changes in the behavior of the liquid at T_λ is the problem that concerns us now.

In explicit calculations of the free energy of vortex lines, we shall assume a simple model in which the particle density is uniform everywhere except in core regions. In a distance of a few angstroms, the density decreases and it reaches zero at the center of a core. We shall assume that the circulation of $\vec{v}_s$ is quantized in the outer region of constant density, as Onsager[55] and Feynman[2] have suggested, so that

$$v_s = b/r \tag{104}$$

there for an isolated straight vortex line bearing one quantum of circulation. The quantization condition gives $b = \hbar/m = 159.0$ m sec^{-1} Å. The units used here are particularly convenient for calculations. The cylindrical radius to the vortex center is r. Later in the discussion we shall describe a method for selecting the velocity at the boundary of a core. If that velocity is known, then the radius of a core can be calculated by Eq. (104). We shall determine the energy of a core approximately for the liquid at 0 °K by a method that is variational, at least in principle. This will be used as an estimate of the core energy even at finite temperatures. The remaining part of the free energy of the liquid containing vortices will be calculated by using the velocity consistent with Eq. (104) and the free-energy values in Fig. 5 or 9.

Let us turn now to the calculation of properties of a vortex core. Consider a sample of liquid ^{4}He at $T = 0$ °K in a cylindrical container of radius R, aligned with the z axis. A rectilinear, quantized vortex state can be defined by the condition that it be an eigenstate of the z component of angular momentum with eigenvalue different from zero.

the liquid to undergo a rearrangement there, per-

We shall be interested in the case where the angular momentum per particle is $\hbar$. An approximate wave function for this state can be written in the form

$$\psi=\prod_{1\leq i\leq N} e^{i\theta_i}P(\rho_i)\psi_0, \tag{105}$$

where (ρ,θ,z) forms a system of cylindrical coordinates. The structure of the wave function ψ is compatible with certain ideas originally discussed by Feynman[2] and later formulated more explicitly by Chester, Metz, and Reatto[53] (CMR). In Eq. (105), ψ_0 is the exact ground-state wave function for the homogeneous system without a vortex, and accounts for the same effects as the correlation function does in ordinary CBF theory without flow. In the present case, it is an eigenstate belonging to the eigenvalue $L_z=0$. The factors of the type $P(\rho_i)$ allow for the variation of the density in the radial direction. Applying the operator L_z to ψ, one can easily verify that ψ belongs to the eigenvalue stated earlier.

If $P(\rho=0)=0$ and $(dP/d\rho)_{\rho=R}=0$, one can use a well-known procedure involving integration by parts to simplify the expectation value of the Hamiltonian with respect to the wave function ψ. The above conditions guarantee that certain surface terms vanish. The result can be expressed more compactly if we write ψ in the form

$$\psi=\prod_{i=1}^{N}\phi(\vec{r}_i)\psi_0. \tag{106}$$

Then defining ϵ by

$$\epsilon=\langle\psi|H-E_0|\psi\rangle/\langle\psi|\psi\rangle, \tag{107}$$

one finds the numerator to be

$$\begin{aligned}\langle\psi|H-E_0|\psi\rangle&=\int\psi^*\left(\sum_{i=1}^{N}-\frac{\hbar^2}{2m}\nabla_i^2+V(\vec{r}_1,\ldots,\vec{r}_N)-E_0\right)\psi\\&\quad\times d^3r_1\cdots d^3r_N\\&=\frac{\hbar^2}{2m}N\int\psi_0^2|\vec{\nabla}_1\phi(\vec{r}_1)|^2\\&\quad\times\prod_{i=2}^{N}|\phi(\vec{r}_i)|^2d^3r_1\cdots d^3r_N.\end{aligned} \tag{108}$$

The number density of particles evaluated at $\vec{r}_1$ is

$$n(\vec{r}_1)=\frac{N\int|\psi|^2d^3r_2\cdots d^3r_N}{\int|\psi|^2d^3r_1\cdots d^3r_N}, \tag{109}$$

and so Eq. (107) may be reduced to

$$\epsilon=\frac{\hbar^2}{2m}\int\frac{n(\vec{r}_1)}{|\phi(\vec{r}_1)|^2}|\vec{\nabla}_1\phi(\vec{r}_1)|^2d^3r_1. \tag{110}$$

If we let $P'(\rho)=dP/d\rho$, then Eq. (110) can be simplified, and

$$\epsilon=\frac{\hbar^2}{2m}\int n(\vec{r}_1)\left[\left(\frac{P'}{P}\right)^2+\frac{1}{\rho_1^2}\right]d^3r_1. \tag{111}$$

Paralleling the procedure in the classical theory of a nonuniform system,[56] one can define a pair distribution function $g(\vec{r}_1,\vec{r}_2)$ by

$$n(\vec{r}_1)n(\vec{r}_2)g(\vec{r}_1,\vec{r}_2)=\frac{N(N-1)\int|\psi|^2d^3r_3\cdots d^3r_N}{\int|\psi|^2d^3r_1\cdots d^3r_N}, \tag{112}$$

and a three-particle distribution function $g(\vec{r}_1,\vec{r}_2,\vec{r}_3)$ by

$$n(\vec{r}_1)n(\vec{r}_2)n(\vec{r}_3)g(\vec{r}_1,\vec{r}_2,\vec{r}_3)=\frac{N(N-1)(N-2)\int|\psi|^2d^3r_4\cdots d^3r_N}{\int|\psi|^2d^3r_1\cdots d^3r_N}. \tag{113}$$

In our further work, we shall approximate ψ_0 by a Jastrow function, and write

$$\psi_0=\prod_{1\leq i<j\leq N}\exp[\tfrac{1}{2}U(r_{ij})]. \tag{114}$$

Applying the Bogoliubov-Born-Green-Kirkwood-Yvon (BBGKY) method, one can generate another useful equation for $n(\vec{r}_1)$ by taking the derivative of Eq. (109) with respect to ρ_1. When Eqs. (105), (112), and (114) are taken into account, one gets

$$\frac{\partial}{\partial\rho_1}\ln n(\vec{r}_1)=2\frac{d}{d\rho_1}\ln P+\int d^3r_2\,n(\vec{r}_2)g(\vec{r}_1,\vec{r}_2)\frac{\partial U(r_{12})}{\partial\rho_1}. \tag{115}$$

Applying $\vec{\nabla}_1$ to both sides of Eq. (112), taking advantage of the fact that $n(\vec{r}_1)$ actually depends only on ρ_1, and making the approximation that

$$g(\vec{r}_1,\vec{r}_2,\vec{r}_3)=g(\vec{r}_1,\vec{r}_2)g(\vec{r}_2,\vec{r}_3)g(\vec{r}_1,\vec{r}_3), \tag{116}$$

one finds that the pair distribution function satisfies the following equation:

$$\begin{aligned}\vec{\nabla}_1\ln g(\vec{r}_1,\vec{r}_2)=\vec{\nabla}_1U(r_{12})&+n_0\int[\vec{\nabla}_1U(r_{13})]g(\vec{r}_1,\vec{r}_3)[g(\vec{r}_2,\vec{r}_3)-1]\,d^3r_3\\&+\int[n(\vec{r}_3)-n_0][\vec{\nabla}_1U(r_{13})]g(\vec{r}_1,\vec{r}_3)[g(\vec{r}_2,\vec{r}_3)-1]\,d^3r_3.\end{aligned} \tag{117}$$

In the case of a uniform liquid, the last integral in Eq. (117) vanishes, and there is a solution of the equation which depends only on r_{12}; then one has $g(\vec{r}_1, \vec{r}_2) = g(r_{12})$. We shall make that approximation in what follows. Later, we shall see that the results of interest here depend only weakly on $g(\vec{r}_1, \vec{r}_2)$, and so it seems likely that only a small error will arise from this approximation. This observation leads to a simplification in numerical work, as we shall now demonstrate. First, multiply both sides of Eq. (117) by $[n_0/(N-1)]g(r_{12})$, take Eq. (116) into account, and then integrate over d^3r_2. Then one finds that

$$\frac{n_0}{N-1}\vec{\nabla}_1 \int d^3r_2\, g(r_{12}) = 0$$

$$= n_0 \int d^3r_2\, g(r_{12})\, \vec{\nabla}_1 U(r_{12}) . \tag{118}$$

Noting that $n(\vec{r})$ is a function only of ρ, one can rewrite Eq. (115) in the following form:

$$\frac{d}{d\rho_1} \ln P^2(\rho_1) = \frac{d}{d\rho_1} n(\rho_1) - \int d^3r_2 [n(\rho_2) - n_0]\, g(r_{12}) \times \frac{\partial U(r_{12})}{\partial \rho_1} . \tag{119}$$

The integrand now involves a short-range factor, and numerical methods can be applied easily in solving the equation. In making estimates, I shall assume

$$U(r) = -(a/r)^5 , \tag{120}$$

and $a = 2.965$ Å. That form of U has been used in a large number of variational calculations[57] dealing with the ground state of homogeneous liquid ^{4}He; the value of a given above was fixed by Francis, Chester, and Reatto[15] by a procedure of that type. For that particular function U, Miller and Woo solved Eq. (117) in the version applicable to a homogeneous liquid,[58] and I have used their results for $g(r)$ in the calculations reported here. Also, I have assumed $n_0 = 0.0218$ atoms Å^{-3}. For the trial functions that we shall work with, there exists some radius R_0 such that $n(\rho) = n_0$ and $P^2(\rho) = 1$ for $\rho > R_0$. Then integrating Eq. (119) from R_0 to ρ gives

$$P^2(\rho) = [n(\rho)/n_0]\, e^{X(\rho)} , \tag{121a}$$

where

$$X(\rho) = \int_\rho^{R_0} d\rho_1 \int d^3r_2 [n(\rho_2) - n_0]\, g(r_{12}) \times \frac{\partial U(r_{12})}{\partial \rho_1} . \tag{121b}$$

In making estimates, we shall assume that $n(\rho)$ has the following form:

$$n(\rho) = \begin{cases} n_0 \sin^2(\pi\rho/2r_0) & \text{for } \rho \leq r_0 \\ n_0 & \text{for } \rho > r_0 . \end{cases} \tag{122}$$

We shall refer to r_0 as the vortex-core radius. This form of $n(\rho)$ was selected mainly because it is mathematically convenient to use, and because it is associated with a function $P(\rho)$ that interpolates smoothly between the points where the behavior is fixed by the boundary conditions, including that at $\rho = 0$. The condition that the wave function, and in turn the density, should vanish at the center of a vortex core has been discussed by Feynman.[2] In a more complete treatment, a more general form of $n(\rho)$ with adjustable parameters could be assumed, and a variational procedure applied. That would be a project of considerable magnitude; so we shall content ourselves with the formula in Eq. (122) in this preliminary study.

The function $n(\rho)$ is plotted in Fig. 12 for the case $r_0 = 4.0$ Å. This value of r_0 is given by Eq. (104) when the velocity is 40 m sec^{-1}. That is the velocity at which the free-energy isotherm terminates for the mean-field model with $\gamma = 0.2$ and at the temperature $T_\lambda = 2.365$ °K, as indicated in

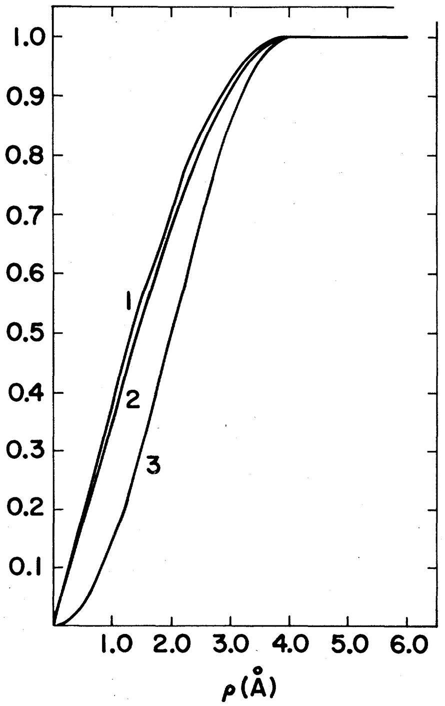

FIG. 12. Vortex core functions vs ρ, the cylindrical radius. Curve 1: $P_0(\rho)$ based on Eq. (121a) with $X(\rho) = 0$. Curve 2: $P(\rho)$ based on Eqs. (121a) and (121b). Curve 3: $n(\rho)/n_0$. For all curves, $n(\rho)$ is given by Eq. (122), and $r_0 = 4.0$ Å.

Figs. 8 and 9. We are now assuming that the size of the core is determined by this velocity for $T=T_\lambda$. It is instructive to neglect the exponential factor in Eq. (121a) now, and thereby obtain a zeroth-order approximation for the solution to Eq. (119); we shall call it $P_0(\rho)$. That function is also plotted in Fig. 12, and one can see readily that if $r_0<R$, where R is the radius of the cylindrical container, then $P_0(\rho)$ satisfies the boundary conditions that were imposed in deriving Eq. (108). In the next approximation, with $n(\rho)$ still given by Eq. (122), the integral in Eq. (121b) was evaluated by numerical methods, and the function $P(\rho)$ was computed from Eq. (121a). The result is plotted in Fig. 12, where it is evident that the correction to $P_0(\rho)$ generated by the factor e^X is small, and the boundary conditions are still satisfied.

The vortex core energy can be computed from Eq. (111) by taking the limits of integration on ρ_1 to be from 0 to r_0. Substituting the zeroth-order function, $P_0(\rho)$, into the equation, one gets integrals that can be evaluated by elementary methods. For unit length of vortex line, one finds the following expression for the core energy ϵ_{c0}, expressed in °KÅ^{-1}:

$$\epsilon_{c0}=\frac{\pi\hbar^2}{mk}n_0\int_0^{r_0}\left[\left(\frac{\pi}{2r_0}\right)^2\cos^2\frac{\pi\rho}{2r_0}+\frac{1}{\rho^2}\sin^2\frac{\pi\rho}{2r_0}\right]\rho\,d\rho\,. \tag{123}$$

After a simple change of variable of integration, one can use the following formulas to evaluate ϵ_{c0}:

$$\int_0^{\pi/2} z\cos^2 z\,dz=\frac{\pi^2}{16}-\frac{1}{8} \tag{124}$$

and

$$\int_0^{\pi/2}\frac{1}{z}\sin^2 z\,dz\approx 1.647\,. \tag{125}$$

The value of ϵ_{c0} is 0.961 °KÅ^{-1}, and it is independent of r_0. It is shown as a horizontal line in Fig. 13, along with the result ϵ_c, which is computed by substituting $P(\rho)$ from Eq. (121a) into Eq. (111) when the upper limit on ρ_1 in (111) is set equal to r_0. The energy per unit length of vortex line associated with the liquid in a cylindrical normalization volume of radius 6.0 Å has also been calculated as a function of core radius. Results are shown in Fig. 13 as curves labeled ϵ_{R0} and ϵ_R.

Calculations parallel to these have been made for models in which $\gamma=0$, that is, for noninteracting elementary excitations. Two cases were studied with the temperature at $T_\lambda=2.415$ °K. In one, the velocity at the core boundary was assumed to be the maximum velocity allowed by a constraint $\sum n_i/N\leq\frac{1}{2}$. Here $\sum n_i$ is the total number of excitations, and N is the number of particles, each of these quantities being referred to unit volume. From Fig. 2, one finds $v_s=44$ m sec^{-1}; and then using Eq. (104), one finds $r_0=3.6$ Å. In the second case, it was assumed $\sum n_i/N\leq 1$, and by a similar procedure it was found that $r_0=3.0$ Å. The energy per unit length of vortex core for each of the three cases is given in the third column of Table I.

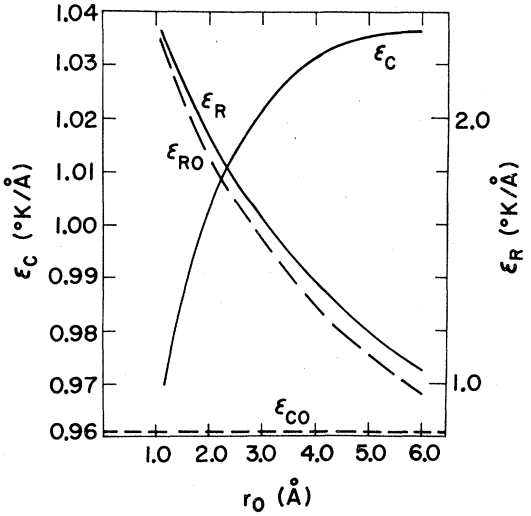

FIG. 13. Energy per unit length of a vortex line vs core radius r_0, for $T=0$ °K. For ϵ_c and ϵ_{c0}, the normalization volume is a cylinder of radius r_0; for ϵ_R and ϵ_{R0} the corresponding radius is 6.0 Å. ϵ_{c0} and ϵ_{R0} are based on the function $P_0(\rho)$; ϵ_c and ϵ_R are based on $P(\rho)$.

The next matter that we shall consider is the calculation of the free energy associated with the flowing liquid outside of the vortex cores for an array of straight, parallel (or antiparallel) vortex lines when the normal fluid velocity v_n is zero. Let us recall that ψ in Eq. (105) serves as the correlation function for excited states in which phonons and rotons are present when there is only one vortex line that is located on the z axis of the coordinate system. The correlation function for a state with many vortex lines can be built up from that in Eq. (105) by including a set of factors of the type shown for each line, provided that θ and ρ are measured with respect to appropriate origins.

TABLE I. Contributions to the free energy of an "antiferromagnetic" vortex array having a lattice spacing of 18.0 Å.

			(°K Å^{-1})		
γ	r_0 (Å)	ϵ_c	F_0	F_a	F_b
0.0	3.0	1.02	−0.52	−0.30	−0.22
0.0	3.6	1.03	−0.38	−0.16	−0.22
0.2	4.0	1.03	−0.43	−0.14	−0.29

In the region we are interested in now, i.e., outside the cores, all factors $P(\rho_i)$ are unity, and the density is constant. Then the fluid velocity computed from the quantum-mechanical current density for ψ is the same as that computed from a velocity potential which satisfies Laplace's equation. The potential is single valued, provided that appropriate branch cuts are introduced. The velocity at any point is clearly the same as that found by assuming the quantization of circulation, with each vortex bearing one quantum unit, and by assuming the superposition principle for combining the contributions from the different lines. It is postulated that the velocity potential computed from the correlation function in that way holds for excited states, and for the system in thermodynamic equilibrium. We shall suppose that the line density is so low that only a minute fraction of the volume of the system is occupied by the cores.

Let $f(v_s)$ be the free energy per particle measured relative to E_0/N, and expressed in °K. It is given by the formula

$$f(v_s) = (1/Nk)[F(v_s) - E_0]\ . \tag{126}$$

The function $F(v_s)$ is the same as that in Eq. (92). The general formula for the free energy associated with the outer region in a vortex array is

$$F_V = n_0 \int f[v_s(\vec{r})]\, d^3r\ . \tag{127}$$

By making a Taylor-series expansion of $F(v_s)$ in Eq. (92), one can show that the leading terms in $f(v_s)$ are as given below:

$$f(v_s) = A + Bv_s^2 + Cv_s^4\ . \tag{128}$$

Explicit expressions for the coefficients that take into account a mean-field interaction are as follows:

$$\begin{aligned} A &= -\frac{1}{k\beta N}\sum \ln(1+n_i)\,, \quad B = \frac{1}{2kN}\left[Nm - \beta\sum n_i(1+n_i)p_{iz}^2\right],\\ C &= -\frac{\beta^3}{24kN}\left(\sum\left[6n_i^2(n_i+1)^2 + n_i(n_i+1)p_{iz}^4\right]\right.\\ &\qquad\left. + \frac{3\beta\gamma\epsilon_0}{N}\,\frac{\left[\sum(2n_i+1)n_i(n_i+1)p_{iz}^2\right]\left[\sum'(2n_j+1)n_j(n_j+1)p_{jz}^2\right]}{1-(\beta\gamma\epsilon_0/N)\sum' n_i(n_i+1)}\right). \end{aligned} \tag{129}$$

Here it is to be understood that the n_i are given by Eqs. (89a) and (89b), but evaluated at $v_s = v_n = 0$. It is easy to show that the bracketed expression in the formula for B is equivalent to the volume times the low-velocity expression for the superfluid density in Landau's theory,[25] when $\gamma = 0$.

Various expressions that others have used for the free-energy density in treating vortices in a rotating container can be derived from $F(v_s)$ evaluated at $T = 0$ °K,[59,60] or at finite temperatures as Taylor-series expressions of $F(v_s)$,[61] or $W(\vec{v}_s, \vec{v}_n)$,[62] where W is the function appearing in Eq. (90). In the last case, one assumes further that $\vec{v}_n = \vec{\omega}\times\vec{r}$, where $\vec{\omega}$ is the angular velocity of the container wall, and $\vec{r}$ is the position vector of a fluid element from an origin on the axis of rotation.

In the range of values of temperature T and coupling constant γ with which we shall be concerned, the coefficients in Eq. (128) have the following properties:

$$A<0\,,\quad C<0\,,$$
$$B\begin{cases} >0 & \text{for } T<T_\lambda \\ =0 & \text{for } T=T_\lambda \\ <0 & \text{for } T>T_\lambda\,. \end{cases} \tag{130}$$

It would be straightforward to evaluate the coefficients by using the results in Eq. (129); however, I have proceeded in a different way for two reasons. The first is that by fitting the approximate form in Eq. (128) to the exact results for $f(v_s)$ at three points that are judiciously chosen, good estimates for the coefficients can be obtained, and the computer results necessary for doing that are already available. The second reason is that in our further work we shall take advantage of the fact that the approximate form in Eq. (128) gives a good fit to the exact expression for $f(v_s)$ over the entire range of the values of v_s that concerns us, that is, up to about 40 m sec^{-1}, and that must be demonstrated explicitly since it cannot be safely inferred just from the properties of a series expansion. Numerical values for the coefficients have been computed only for $T \approx T_\lambda$, since that is what is needed in our further work. For $\gamma = 0.0$, the coefficients were evaluated for $T = 2.40$ °K, which is just 0.015 °K below T_λ, by requiring that the values of $f(v_s)$ determined by the formula in (128) agree with exact values of $f(v_s)$ at $v_s = 0.0$, 20.0, and 40.0 m sec^{-1}. When $f(v_s)$ is expressed in °K/atom and v_s in m sec^{-1}, the coefficients are $A = -0.3425$, $B = 1.807\times10^{-5}$, and $C = -0.9643\times10^{-7}$. For $\gamma = 0.2$ the coefficients were evaluated for 2.35 °K, which again is just 0.015 °K below T_λ for that value of γ. In this case, the exact match was made at $v_s = 0.0$, 18.0 and 36.0 m sec^{-1}. The coefficients were computed to be $A = -0.3187$, $B = 1.680 \times 10^{-5}$, and $C = -1.270 \times 10^{-7}$. The free-energy curves reconstructed from the computed coefficients are compared with the exact results in Fig. 14. One can see there that over a large range of v_s, there is no discernible difference between the original and reconstructed curves, at least on the scale used in the figure, and that it is reasonable to use the approximate functions to make estimates. To very good approximation, the values of A and C at T_λ are the same as those given above. For the value of B at T_λ, we shall use the exact result, viz., zero. The simple approximate formula for $f(v_s)$ at T_λ which follows from these considerations has important consequences for our analysis because it leads to integrals for the energy of a vortex array which can be evaluated easily, and because it enables us to understand some qualitative features of the free energy of an array. At the same time we are assured that only minor errors are introduced by the truncation procedure.

In dealing with a vortex array, it is useful to consider an elementary problem involving just two straight, parallel vortex lines separated by a distance R, as in Fig. 15. Using the law of cosines, one can easily show that the following relation holds for the angles indicated in the figure:

$$\cos\theta' = \frac{\rho\cos\theta - R}{(R^2 + \rho^2 - 2R\rho\cos\theta)^{1/2}}. \tag{131}$$

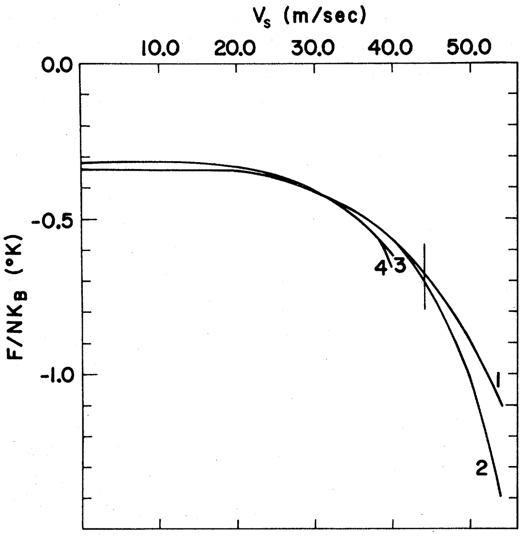

FIG. 14. Free energy per particle as a function of superfluid velocity v_s when $v_n = 0$. Exact functions are evaluated using Eq. (92); reconstructed functions are based on Eq. (128). For $\gamma = 0.0$: curve 1, reconstructed; curve 2, exact. For $\gamma = 0.2$: curve 3, reconstructed; curve 4, exact.

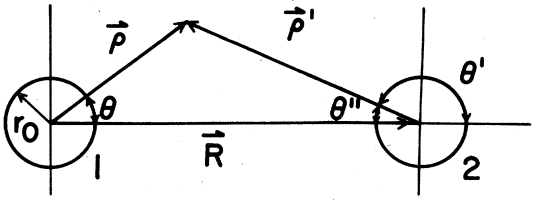

FIG. 15. Pair of straight, parallel vortex lines.

It is then straightforward to derive the following formulas:

$$\left(\frac{\partial\theta'}{\partial\rho}\right)_\theta = -\frac{R\sin\theta}{\rho}, \tag{132a}$$

$$\left(\frac{\partial\theta'}{\partial\theta}\right)_\rho = \frac{1}{2}\left(\frac{1}{2} - \frac{R^2 - \rho^2}{\rho'^2}\right). \tag{132b}$$

Let us assume that each vortex line bears one quantum of circulation. Then the velocity potential associated with the vortex at position 1 is $b\theta$; the potential for the vortex at position 2 is $b\theta'$. The velocity fields derived from them are

$$\vec{v}_1 = \vec{\nabla}_1 \theta = (b/\rho)\,\hat{\theta}, \tag{133a}$$

and

$$\begin{aligned} \vec{v}_2 &= \vec{\nabla}_2 \theta' = (b/\rho')\,\hat{\theta}' \\ &= \vec{\nabla}_1 \theta' = \frac{b}{\rho}\left(\frac{\partial\theta'}{\partial\theta}\right)_\rho \hat{\theta} + b\left(\frac{\partial\theta'}{\partial\rho}\right)_\theta \hat{\rho}. \end{aligned} \tag{133b}$$

Reversing the sense of rotation of a vortex implies that its velocity potential changes sign.

For an array, one can calculate the total velocity at any point in the outer region by using Eqs. (132) and (133) and forming a vector sum with contributions from all of the vortices. Because the coefficient C in Eq. (128) is negative near T_λ, it seems intuitively than an array likely to produce a large negative contribution to the free energy will be close packed and "antiferromagnetic." A picture of such an array can be visualized as follows. Start with a set of circles of radius $\frac{1}{2}R$ whose centers are separated by a distance R on a horizontal line. All vortices on this line have the same sense of rotation. Just above it place another line of similar circles, displaced horizontally so that each one just touches two circles on the line below. The sense of rotation of any vortex on the second line is opposite to that of the vortices on the first line. Repeating this prescription, one forms an infinite "antiferromagnetic" array of vortices, and it has the spatial structure of the base plane of a hexagonal-close-packed lattice. Since nearly all of the area lies inside of the circles, one can obtain a good estimate of the free energy for the outer region by integrating v_s^4 for a single circle and then multiplying by an appropriate constant. If we focus on a specific vortex, then the centers of its nearest neighbors lie on the vertices of a hexagon. The second- and third-nearest neighbors form the next smallest hexagonal ring. The fourth- and fifth-nearest neighbors form the third-smallest hexagonal ring. The integral of v_s^4 over the portion of the central circle with $\rho > 5.0$ Å, taking into account contributions from the central vortex and those from successive hexagonal rings as described above, is shown in Fig. 16. The integral appears to be converging in an oscillatory manner as successive rings are added. It seems likely that the value of the integral for an infinite number of rings will lie between curves 2 and 3 in Fig. 16, and that its peak will occur when $R \approx 18$ Å. Then the lowest value of the free energy associated with the outer region will occur for this spacing. In making estimates, we shall work with curve 3 in Fig. 16. Multiplying those values by $n_0 C$, one obtains part of the free energy per unit length of vortex line, which we shall call F_b.

If this "antiferromagnetic" array were infinite, then at the center of each vortex the resultant velocity due to all *other* vortices would be zero. This follows from a symmetry of the array associated with reflection through an origin taken on any vortex. Hence, under the assumption that the Helmholtz theorem holds, the array would be stationary.

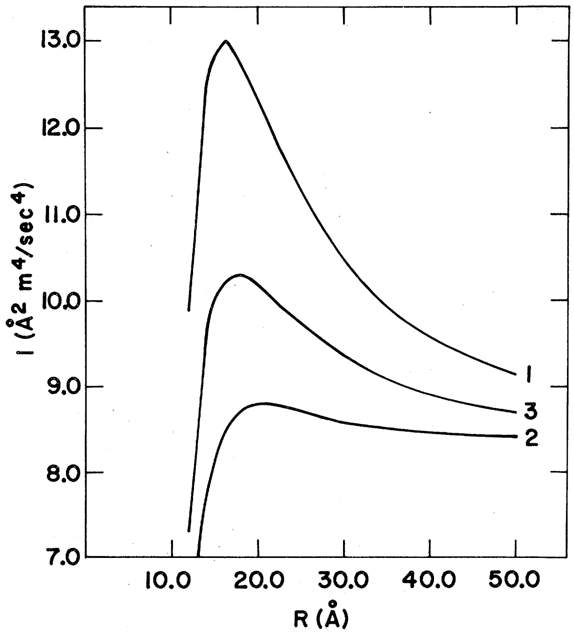

FIG. 16. I is the integral of v_s^4 over a plane annular region with $5.0\ \text{Å} < \rho < \frac{1}{2}R$, for an "antiferromagnetic" array of straight vortex lines. Curves 1, 2, and 3 are based on contributions from neighbors included in successively higher hexagonal rings, together with the contribution from the central vortex. v_s was computed with the aid of Eqs. (132) and (133).

The cores, however, become distorted from circular shapes because of the influence of the members of the array on each other. For the case we are considering, computer calculations indicate that for a spacing of about 20 Å and core radii of about 3–4 Å, the maximum distortions are of the order of 0.5 Å in the radii. Let us recall in this connection that a core boundary is assumed to be determined by the condition that a certain specified velocity is reached. A rather elaborate calculation would be needed to treat the distortions accurately. However, because of the manner in which a core boundary is determined, one can obtain a reasonable estimate of the contribution to the free energy in the outer region between r_0 and 5.0 Å by supposing that the velocity is just that due to the central vortex. The quantity F_a is the part of the free energy per unit length obtained by multiplying the integral of v_s^4 for this annular region by $n_0 C$. The free energy per unit length associated with the outer region of a vortex within a circle of radius $\frac{1}{2}R$ is $F_0 = F_a + F_b$. These quantities have been evaluated for noninteracting vortices, where $\gamma = 0.0$, and for the mean-field case where $\gamma = 0.2$. The results for a particular lattice spacing are shown in Table I, along with the vortex core energy taken from Fig. 13. No attempt has been made to adjust the core energy to take distortions into account. The term involving A in Eq. (128) has been neglected because its contribution is not changed by the presence of vortices. In the table, one can see that F_0 and ϵ_c tend to cancel, and their magnitudes differ by a factor of about 2 or 3, depending on the specific parameters that were used. The sum $F_0 + \epsilon_c$ is found to be positive in every case we have examined. So taken at face value, the results indicate that the rest state is thermodynamically preferred over states with vortices by virtue of having lower free energy at the temperature T_λ. However, opposing terms in the free energy are close enough in magnitude that one should seriously consider the possibility that a more accurate calculation of the core energy and treatment of a wider class of vortex arrays would lead to the opposite conclusion.[63] It is clear that if vortex states are found to have the lower free energy at T_λ, then they will also have lower free energy for some smaller temperatures because the coefficients in Eq. (128) are continuous functions of temperature.

The possibility that vortex rings start to condense in the liquid, perhaps as arrays, at a temperature that is somewhat below T_λ is a matter that should be examined closely. It is interesting to speculate that the change in the free-energy function $F(v_s)$ at T_λ, associated with the change in sign of B in Eq. (128), causes vortex rings in haps even coalescing into vortex lines. This activity could then produce a specific-heat anomaly. These ideas are compatible with conjectures made long ago by Onsager[55] and Feynman.[2] In Sec. III we saw that the change in behavior of $F(v_s)$ at T_λ may cause the transition to superfluidity. So the simultaneous divergence of the specific heat and the transition in hydrodynamic properties may be due to the change in character of the Helmholtz potential.

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[63] Since the time that this paper was submitted for publication, it has been shown that if the free energy per particle outside the vortex cores has the qualitative features as a function of v_s and T shown in Figs. 5 and 9, then there definitely exist configurations of vortex rings that have lower free energy than the system at rest for a range of temperatures starting somewhat below T_λ. For details see G. McCartor and H. W. Jackson, J. Low Temp. Phys. 31, 313 (1978).