UCRL-11541

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PART I. APPLICATIONS OF THE VARIATIONAL PRINCIPLE TO STATISTICAL MECHANICS

PART II. SOME PROPERTIES OF He^3

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Research and Development

UCRL-11541

UNIVERSITY OF CALIFORNIA

Lawrence Radiation Laboratory
Berkeley, California

AEC Contract No. W-7405-eng-48

PART I. APPLICATIONS OF THE VARIATIONAL PRINCIPLE TO STATISTICAL MECHANICS

PART II. SOME PROPERTIES OF He^3

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(Ph. D. Thesis)

July 13, 1964

PART I. APPLICATIONS OF THE VARIATIONAL PRINCIPLE TO STATISTICAL MECHANICS

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ABSTRACT

Part I.

The variational approaches in statistical mechanics are discussed. The relationships among several formalisms and possible simplifications are pointed out.

The principle is applied to the equation of state of gas-liquid, the Ising model, and the Boson system above the transition temperature. No essentially new results are obtained, but through these simple examples, it is seen how to use the variational principle to make a thermodynamically consistent approximation and how to obtain the stable solutions.

Part II.

Some equilibrium properties of He^3 are calculated by using thermodynamical Green's function formalism. The T-matrix integral equation is solved by neglecting the statistical factor in the intermediate states and using the effective mass approximation.

The effective mass and ground state energy are calculated and the correction due to the statistical factor is estimated.

I. INTRODUCTION

Among various ways of doing calculations of the many-body problem, one of them uses equations of motion (or the Green's function formalism) which usually neglects multiple-particle correlation in order to solve the chains of integral equations. Many other approximations are based on physical arguments in different kinds of problems, for instance, the Bruckner reaction matrix method, Landau's theory, generalized H-theorem, and R. Peierls' variational principle. It is the purpose of this first part to show that all the methods mentioned are essentially the same variational approach with different approximations.

We first review the so-called "variational principle" in the literature and show the relationship among these various approaches. Actually, here is a very general way of calculating the self-energy of single particles in the system by using the variational principle derived by Luttinger and Ward. It seems, however, extremely hard to carry out in any realistic problem. The simplified way is to use the quasi-particle approximation, assuming that the system consists of interacting quasi particles which are defined in different ways in different systems.

It is pointed out that one of the advantages of using a variational approach is that it helps one to decide whether or not the approximation used will give an acceptable answer.

In III. A the principle is applied to the gas-liquid system.

The Hartree approximation is made, but as the total volume is reduced because of the hard core of the molecules, a curve of Van der Waal's type is obtained. The thermodynamical stability condition gives us a prescription for discarding certain solutions that gives the usual curve of the equation of state.

III. B is the application to the Ising Model. A trial solution that does not include correlation among particles at different sites is the well-known Bragg-Williams zero approximation. If we start with a wave-type solution (similar to spin wave in ferromagnetism) it is better, since the free energy is lower than the first solution, but it does not illustrate the differences due to dimensions of the system. If "right" states are chosen at first, one obtains the exact solution of the one-dimensional problem with no magnetic field, but the extension of it to two dimensions is almost impossible because of the complicated combinatorial factor associated with the counting of the states.

III.C is a brief note to show that a self-consistent Hartree approximation is not stable on the basis of the phase shifts given by usual potentials studied in the literature.

II. GENERAL THEORY

Several works on this subject are briefly reviewed in this chapter. First, R. E. Peierls' variational principle, and papers by Girardeau,[1] Cohen[2,3] and Riesenfeld and Watson.[4] Later, we show that the most general form is contained in Luttinger and Ward's paper.[5] The usual applications mentioned above take only terms of the first order. One of the advantages of putting the calculations of the statistical mechanics in variational form is that consistency, which will be discussed later, is assured, and, furthermore, the method indicates where the approximation breaks down.

The general theory is hard to carry out at finite temperature, and a quasi-particle approximation is suggested. It is simpler, but it cannot be mathematically justified; only the success of its application gives the physical picture of the system considered and the validity of our approximation.

The variational principle for statistical mechanics, which is best understood in terms of the extension of the variational calculation of eigenvalues of the Schrödinger equation, should be attributed to R. E. Peierls, who derived it thirty years ago. It has recently been extensively applied to the many-body problem.[1] The principle is extremely simple.

$$Z = \sum_{\alpha} \langle\alpha|\exp\left[-\beta(H - \mu N)\right]|\alpha\rangle \geqq \sum_{\alpha} \exp\left[-\beta\langle\alpha|H - \mu N|\alpha\rangle\right] \equiv Z_{var} , \tag{1}$$

where H = total Hamiltonian, μ = chemical potential, and F_{var} = free energy = $-\beta^{-1} \ln Z_{var}$; with $\beta^{-1} = kT$; then $Z = Z_{var}$ only if α is the true wave function of the N-particle system.

The usefulness of (1) is that though it is almost impossible to evaluate $\langle\alpha|\exp\left[-\beta(H - \mu N)\right]|\alpha\rangle$, it is easier to calculate $\langle\alpha|H - \mu N|\alpha\rangle$ when α is an arbitrary state vector which may contain some variational parameters. The essential features of the system are contained in F_{var} if α is properly chosen. For instance, in a condensed Boson system we would use $\alpha_i = (\eta_i)^{-\frac{1}{2}}(a_k^+)^{\eta_i}|0\rangle$, where η_i takes on all possible integer values and a_k^+ is a phonon creation operator. The result of this formalism is the same as the result "pair Hamiltonian" formalism. This is rather natural, since in (1) , all off-diagonal elements in α representation are neglected. Applying this formalism to a superconducting system, we can derive BCS theory.[6] Even though we might at first think that the usual problems that are to be solved can also be framed into this theory, it is actually not possible when more involved calculations are attempted. Certainly, it should be argued that more elaborate trial-wave functions will provide all results that can possibly be derived from other methods, but the discussion is beyond what we can include here. Basically, this variational approach cannot be better than the Hartree-Fock approximation. As a matter of fact, they both give the same equation for the

free energy.

It is derived in Ref. 1:

$$F_{var} = \pm \beta^{-1} \ln(1 \mp f_i) - \frac{1}{2} W_{ij} f_i f_j W_i ,$$

where W_i W_{ij} are the kinetic and potential energy in certain specific representations, and the distribution function is

$$f_i = \frac{1}{\exp \beta(W_i + W_{ij} f_j) \pm 1} ,$$

which is to be solved for f_i. In the Hartree-Fock approximation, all the equations are the same.

The so-called "self-consistent" method is actually the same approximation; so is the generalized H -theorem.[4] Let us see from the entropy

$$TS = -\beta^{-1}\left[f_k \ln f_k \mp (1 \pm f_k) \ln(1 \pm f_k)\right]$$

the total energy

$$u = \sum_k \frac{k^2}{2m} f_k + \frac{1}{2} \sum f_k f_{k'} \left[V(0) \pm V(k - k')\right], \tag{3}$$

where f_k is the distribution function of particles with momentum k, $v(k)$ the Fourier transform of potential. Using

$$\delta F = \delta(U - TS - \mu N) = 0,$$

we obtain

$$f_k = \left[\exp \beta(k^2/2m + f_{k'}(V(0) \pm V(k - k') - \mu) \mp 1\right]^{-1},$$

and

$$F = \pm\beta^{-1} \sum_k \ln(1 \mp f_k) - \frac{1}{2} \sum_{kk'} (V(0) \pm V(k - k')) f_k f_{k'} . \tag{4}$$

It is not surprising that this answer is the same as we obtain from Eq. (2), since correlation is neglected in (3), and (4) is the consequence with only statistics taken into consideration. Similarly, the generalized self-consistent[2,4] approximation as it is used is also a variational approach. It differs from the above formulation only in that a parameter ξ is introduced, so that

$$\text{total energy} = \sum k^2/2m\, f_k + \frac{\xi}{2} \sum f_k f_{k'} v(\chi) \pm v(h - h')$$

$$+ \frac{1 - \xi}{2} \sum F_{kk'} \left[v(0) \pm v(h - h')\right],$$

where $F_{kk'}$ is the two-particle density matrix; if $\xi = 0$, u is exact; if $\xi = 1$, the approximation is the Hartree Fock approximation. With the u given above, and requiring $\frac{\delta F}{\delta f_k} = 0$, we then have

$$\frac{dF}{d\xi} = \frac{1}{2} \sum_{kk'} (f_k f_{k'} - F_{kk'})(V(0) \pm V(k - k')) \tag{5}$$

when f_k and $F_{kk'}$ depend on ξ. This formulation is said to be useful for the calculation of properties of electron gas at intermediate densities, but in practice, finding $\delta F/\delta f_k = 0$ with $F_{kk'}$ unknown is very hard, and any approximation with $\delta F/\delta f_k = 0$ not satisfied will lead to a thermodynamical inconsistency (which will be discussed later).

Though some important problems can be solved approximately in the formalism mentioned above, it is by no means general, and is very hard to generalize. Furthermore, it is perhaps easier to do variational calculations if we can write down the total energy and entropy and vary $F = U - TS - \mu N$, but actually entropy is much harder to calculate from $\mathrm{Tr}\, \rho \ln \rho$ than from $F = \mathrm{Tr}\, \rho$. Unless some approximation is used, it is hard to start with $F = U - TS - \mu N$ and, generally speaking, entropy is physically clear only in some simple system. Recently several people have established the

expansion for free energy, in terms of either the single-particle Green's function[5] or occupation number in momentum space.[7] Since the expansion given in Ref. 5 is the general expression for free energy, which is shown to satisfy a variational principle, it can be used even in practical calculations where some approximation is made to include only a sweries of specialized diagrams.

We sketch the theory given in Ref. 5 to indicate how it can be used. Free energy can be written as

$$-\beta^{-1} \sum_{r} \sum_{\ell} \exp(\zeta_\ell 0^+) \Big\{ \ln(\epsilon_r + G_r(\zeta_\ell) - \zeta_\ell) \times (\zeta_\ell - \epsilon_r - G_r(\zeta_\ell))^{-1} G_r(\zeta_\ell) \Big\} + Y' ,$$

where r denotes the quantum number and specifies the states, and ζ_ℓ may be an even or odd integer depending on whether we have bosons or fermions. The $G_r(\zeta_\ell)$ are the proper self-energies, which are given by all linked closed diagrams with one line removed. We do not give here the rules of calculating "closed linked diagrams," which are given in Ref. 5. If we define skeleton diagrams as diagrams with no self-energy part, then $G_r(\zeta_\ell)$ are the contributions from all closed linked skeleton diagrams with propagator $\frac{1}{\zeta_\ell - \epsilon_r - G_r(\zeta_\ell)}$, instead of $\frac{1}{\zeta_\ell - \epsilon_r}$, and with one line opened. Y' is the contribution of closed-skeleton diagrams. It is shown in Ref. 5 that

$$\frac{\delta Y'}{\delta\, S_r(\zeta_\ell)} = G_r(\zeta_\ell)\,,$$

$$S_r(\zeta_\ell) \equiv \left[\, \zeta_\ell - \epsilon_r - G_r(\zeta_\ell) \,\right]^{-1} \tag{6}$$

if and only if $\frac{\delta}{\delta\, G_r(\zeta_\ell)}$ (free energy) $= 0$. Equation (6) actually is a complicated integral equation which determines $G_r(\zeta_\ell)$, since Y' is independently given. Furthermore (6) has to be satisfied to guarantee thermodynamical consistency.[8]

In practice, (6) cannot be carried far, and only the Hartree-Fock solution, which takes $\frac{1}{2}$ as y', has been investigated; this procedure is equivalent to Peierls' variational principle, as we have indicated before. Numerically, even the H-F approximation is already too difficult to solve, not to say the random-phase approximation and the T approximation. Usually, all these approximations are not consistently calculated, and therefore some thermodynamical equalities are not satisfied; for instance, the entropy thus calculated is not the same as the derivative of free energy, and the theorem of Hugenholz-Van Hove will be violated.[8] Since (6) is too formidable to handle, we ask what one can do if the properties of a many-particle system at finite

temperature are wanted and self-consistency is required. In Eq. (6), Y' can be an arbitrary number of diagrams, and the consistency is still maintained. In practice, (6) can hardly be solved, if more terms than the Hartree-Fock approximation are included.

We define f as the quasi-particle distribution function for convenience, and take it in momentum space. (Whether the quasi particle so defined will describe the system very well is another problem.) Entropy is given by

$$TS = -\beta^{-1} \mathrm{Tr}\left[f \ln f \pm (1 \mp f) \ln(1 \mp f) \right];$$ in a uniform system the distribution function is diagonal in momentum space,

$$N = \sum_k f_{kk},$$

and the total energy $$U = \sum_k \frac{k^2}{2m} f_{kk} + Y'.$$

Y' will consist of all the diagrams that we need to keep in order to make a good approximation; then we put $\delta F = \delta(U - TS - \mu N) = 0$,

$$f_k = \left[\exp \beta\left(\frac{k^2}{2m} + \Sigma(k) - \mu \right) \pm 1 \right]^{-1}$$

and

$$\Sigma(k) = \frac{\delta Y'}{\delta f_k}. \tag{7}$$

Thus, for instance,

$$S = \left(-\frac{\partial F}{\partial \beta}\right)_{\mu, v} = -(T\beta)^{-1}\left[f_k \ln f_k \pm (1 \mp f_k)\ln(1 \mp f_k)\right]$$

as it is defined.

Furthermore, (7) guarantees that the Hugenholz-Van Hove theorem is satisfied. It should be emphasized that f_k does not have direct physical meaning, unless the U and S calculated are good enough to justify saying that the whole system is described by quasi particles with a distribution function f_k.

The choice of y' is not easy. In the exact expression (6), it is well defined, but in the approximate calculation, y' is chosen according to whether it yields good results for total energy or not. Furthermore, the validity of the quasi-particle approximation depends on the nature of our approximation also. Bruckner's reaction-matrix approximation can serve as a good example. First, we know that in his calculation the imaginary part of the self-energy is neglected, and the correction was made later. The correction term is proportional to higher powers in the R matrix. If this kind of calculation is extended to finite temperature, we write down the entropy and energy as before, with y' consisting of all ladder diagrams in his calculation. Our way of writing entropy or justifying the quasi-particle concept depends on whether or not higher powers in the R reaction are really small. Furthermore, it shows the

difficulty of extending the calculation to finite temperature; that is, several important quantities, such as rearrangement energy and renormalization factors, are most likely very important, but a consistent calculation is perhaps too formidable.

One of the advantages to applying the variational principle is that not only is it an approximation, but it also provides an indication of where it breaks down. It means $\frac{\delta F}{\delta \rho_k} = 0$ is the equation from which one obtains ρ_k, but any acceptable solution must also satisfy $\frac{\delta^2 F}{\delta \rho_k \delta \rho_k} > 0$ to insure the stability of the solution. The sign of $\frac{\delta^2 F}{\delta \rho_k \delta \rho_k}$ is discussed in the Hartree-Fock approximation in Ref. 9; we take free energy F in (3), then

$$\delta^2 F = \beta^{-1} \sum \delta\rho_{k_1} \frac{1}{\rho_{k_1}} \frac{1}{1 \pm \rho_{k_1}} \delta\rho_{k_1} + \sum \delta\rho_{k_1} \left[V(k_1 - k_2) \pm V(0) \right] \delta\rho_{k_2} . \tag{8}$$

To discuss the sign of this quadratic, one needs to know the eigenvalues of the matrix $\| C_{kk'} \|$, where

$$C_{kk'} = \beta^{-1} \frac{1}{\rho_k} \frac{1}{1 \pm \rho_k} \delta_{kk'} + \left[V(0) \pm V(k - k') \right].$$

Unless all eigenvalues are positive, $\delta^2 F$ will not be positive for all $\delta\rho_k$.

To discuss (8) even in simple approximations is not easy, not to mention more complicated approximations, but whenever an approximation is made, it is necessary to examine $\delta^2 F$. Though $\delta^2 F$ in the general form is always too hard to see, it would be much simpler if $\delta\rho$ were specified as $\delta\rho = \frac{d\rho}{d\mu} d\mu$, then (8) would be easy to calculate. If $\delta\rho$ is fixed this way, the sign $\delta^2 F$ in (8) is the same as $\frac{\partial N}{\partial \mu}$, and $-\frac{\partial P}{\partial V}$ must be positive. It seems that perhaps it is not necessary to carry out the general discussion. Instead, we may only have to know whether or not thermodynamical stability is satisfied.

III. APPLICATION

In this chapter, the variational principle is applied to three problems. First, we consider the gas-liquid phase transition. Equations of state for the gas and liquid are obtained by simple calculations which are only a consistent Hartree approximation. We also show that the solution derived from the variational principle in some region is not acceptable, and this breakdown indicates a phase transition. Though it is not a theory for the phase transition, it provides a criterion for calculation.

The variational principle is applied to the Ising model. It does not simplify the problem. We can solve only the one-dimensional problem and show how the "quasi particle" that we pick up to calculate the property of the system will influence our results. The phase transition in the Ising model is due to long-range correlation, and wrong conclusions can be drawn if an approximation which takes no consideration of this point is used, and vice versa.

In the last section, we discuss the calculation of the Boson system, He^4, above transition temperature. It is shown, from the point of view of variational principle, that the existing calculations on the subject are not to be accepted. It needs more elaborate consideration than using the Hartree-Fock approximation with the effective interacting potential given by the phase shifts. Some possible improvements are suggested.

A. A Discussion of the Equation of State

The equation of state is not easy to calculate in general. It is a matter simple in principle but complicated in practice. The discontinuity in the equation of state, or the phase transition, has been the concern of physicists for many years. Until Onsager's exact solution of the two-dimensional Ising model, it was even doubted whether starting from first principles, the phase transition would appear automatically.[10]

Generally speaking, there are two ways of approaching the problem. In the early works,[11] the system is assumed to consist of several components to explain the mechanism of phase transition, and discontinuity shows up naturally as the Gibb's function of different components have different values. Certainly we do not regard this approach as theory. Another approach examines the free energy directly; for instance, the method of cluster expansion. Some remarkable progress has been made concerning the relationship of the phase transition with the force between interacting particles. However, we know that force is not the only thing important in phase transition. The weighting factor may also play a decisive role. Bose-Einstein condensation is an example. To sum up, a unified approach really does not exist in the theory of phase transition.

It is not our intention to discuss the theory of phase transition.[10] The question is how, with a given two-particle potential, to calculate the equation of state. Since we realize it

is impossible to present a way which might be applicable for all kinds of systems, different systems must have different approximations. Here is the simplest application.

As far as the gas-liquid phase transition is concerned, it is the type of the force which is responsible. We know the Hartree approximation is reasonably good for long-range, weak potentials, but certainly breaks down for the infinitely strong, short-range force which exists in molecules. Since the interaction considered is weak except for the hard core, we expect all particles having a certain momentum k to move in a self-consistent field.

Because of the hard core one needs to take higher and higher powers of the potential (essentially the ladder diagram) to arrive at almost the same solution of the pseudo-potential method. As we have shown, we do not have much difficulty in obtaining the same result. It will be advisable to give the physical arguments of how to write a reasonably good two-particle density matrix in terms of ρ_1 :

$$\langle 12|\rho|1'2'\rangle = \mathrm{Tr}\ \langle \psi^{+}(1)\psi^{+}(2)\psi(1')\psi(2')\rho\rangle$$

$$= \int \rho_2(k,k',\bar{k})\, e^{i\bar{k}(R-R')}\, e^{ik(r_1-r_2)}\, e^{-ik'(r_1'-r_2')}\, \frac{d^3\bar{k}\, d^3k\, d^3k'}{(2\pi)^9} .$$

Here

$$\rho_2(\underset{\sim}{k}, \underset{\sim}{k}', \bar{\underset{\sim}{k}}) = \mathrm{Tr}\,\langle \psi^+\left(\frac{\bar{\underset{\sim}{k}}}{2} - \underset{\sim}{k}\right)\psi^+\left(\frac{\bar{\underset{\sim}{k}}}{2} + \underset{\sim}{k}\right)\psi\left(\frac{\bar{\underset{\sim}{k}}}{2} - \underset{\sim}{k}'\right)\psi\left(\frac{\bar{\underset{\sim}{k}}}{2} + \underset{\sim}{k}'\right)\rho\rangle$$

and

$$\underset{\sim}{R} = \frac{1}{2}(\underset{\sim}{r}_1 + \underset{\sim}{r}_2), \quad \underset{\sim}{r} = \underset{\sim}{r}_1 - \underset{\sim}{r}_2 \; ; \qquad \rho = e^{\beta(H - \mu N)} .$$

Here $\langle\ \rangle$ is used to denote the ensemble average, $\bar{k}$ the total momentum, and k, k' the relative momenta of the incoming and outgoing particles. In the region where $R \leqslant a$, $R' \leqslant a$, the a is the radius of the hard core; $\psi(1)$, $\psi(2)$ do not overlap. Several ways can be used to say the same thing, namely, the integration of R does not extend to whole space V; rather $\sim (1 - Na^3)$. This is a very important factor for obtaining in order to obtain the discontinuity in the phase transition. If the interaction is weak and is not strongly dependent on the density of the system, then the whole system will reduce its volume continuously to zero. It is the term $(1 - Na^3)$ which forces changes of the structure of the system to take place when the volume is sufficiently reduced, comparable to Na^3.

If $\rho_2(k, k', \bar{k})$ is independent of $\bar{k}$ and set equal to $\rho(k)\rho(k')$ in the Hartree approximation, there should be another consideration, viz., integration over R (or R') should not be

extended through the whole space as argued before. The result is the same as using the variational principle in (4) $\delta F = 0$, $F = U - TS + \mu N$. The potential in momentum space is given as

$$\langle k_1 - k_2 | v | k_1 - k_2 \rangle = -\left[\alpha + \beta'(k - k_2)^2\right]\frac{1}{V}$$

when $k_1 k_2 \leqslant k_0$, and $\langle v \rangle = \gamma \frac{1}{V}$ when $k_1 k_2 \geqslant k_0$; α, β', γ, k_0 are all constant. More complicated potentials will obscure our discussion. Also, this potential does give the essential featurs of any realistic potential of the type with hard core and weak attractive tail.

We use the H-F approximation $\rho_2(k_1 k_2) \approx \rho_1(k_1)\, \rho_1(k_2)$, but we must account for the hard-core effect. It is included simply by reducing the volume of the whole system

$$\rho_2(k_1 k_2) = (1 - a\frac{N}{V})\, \rho_1(k_1)\rho_1(k_2) .$$

Our phase-space integral element is

$$dw_p = \frac{eV}{N}\frac{d^3p}{(2\pi)^3}$$

and

$$V =$$

$$U = N \int \frac{k^2}{2m} \rho_1(k)\, dw_k + \frac{N(N-1)}{2}$$

$$\times \int \langle k_1 - k_2 | v | k_1 - k_2 \rangle \rho_1(k_1) \rho_2(k_2) dw_{k_1}\, dw_{k_2}\, (1 - a\frac{N}{V}) ,$$

$$TS = -\beta^{-1} \int \ln \rho_1(k) \cdot \rho_1(k)\, dw_k ,$$

$$N = N \int \rho_1(k)\, dw_k .$$

Use

$$\delta F = 0,$$

and

and $\rho_1(k)$ depends on k as follows:

$$\rho_1(k) = A(k) \quad \text{for} \quad k \leqslant k_0 ,$$
$$= B(k) \quad \text{for} \quad k \geqslant k_0 ,$$

$$A(k) = e^{-1} e^{-\beta\left[k^2/2m + (1 - a\rho)(\alpha\rho_1 + \beta'\bar{\rho}_1 + \beta' 1^2 \rho_1)\right]} + \mu/kT ,$$

$$B(k) = e^{-1} e^{-\beta\left[k^2/2m + (1 - a\rho)\gamma\rho_2\right]} + \mu/kT .$$

Here

$$\int_0^{k_0} A(k) \frac{d^3k}{(2\pi)^3} = \rho_1 ,$$

$$\int_0^{k_0} A(k)\, k^2 \frac{d^3k}{(2\pi)^3} = \bar{\rho}_1 ,$$

$$\int_{k_0}^{\infty} \beta(k) \frac{d^3k}{(2\pi)^3} = \rho_2 ,$$

$$\rho = \frac{N}{V}$$

and ρ_1, $\bar{\rho}_1$, ρ_2 are to be determined consistently from the equations

$$F/kT = -\int dw_p\, \rho_1(p) - \frac{1}{2} \frac{N(N-1)}{2} \langle k - k' | V | k - k' \rangle\, \rho_1(k)\rho_1(k') dw_k dw_{k'}$$

and

$$PV = -F = NKT(1 - a\rho)\left\{1 - \frac{1}{2}\rho\left[(\alpha\rho_1^{\,2} + \beta'\rho_1\bar{\rho}_1) - \gamma\rho_1^{\,2}\right]\right\} . \tag{9}$$

The second term is the correction to an ideal gas, and PV is not an infinite series of ρ or $\frac{N}{V}$ which diverges at the point of condensation, as is discussed in the theory of cluster expansions.

We realize the simplicity of (9) is due to our approximation in $V(k - k')$, but the point that we want to make is how to obtain the equation of state from the variational point of view:

$$\rho_1 = \int_0^{k_0} A(p) \frac{d^3p}{(2\pi)^3} = e^{-1} e^{\mu/kT + \frac{1}{kT}(1 - a\rho)(\alpha\rho_1 + \beta'\bar{\rho}_1)}$$

$$\times \int_0^{p_0} e^{-p^2/2m^*kT} \frac{d^3p}{(2\pi)^3}, \tag{10}$$

$$\frac{1}{m^*} = \frac{1}{m} - (1 - a\rho)\beta'\rho,$$

$$\bar{\rho}_1 = e^{-1} e^{\mu/kT} e^{\frac{1}{kT}(1-a\rho)(\alpha\rho_1+\beta\bar{\rho}_1)} \int_0^{p_0} p^2 e^{-p^2/2m^*kT} \frac{d^3p}{(2\pi)^3} \tag{11}$$

$$\rho_2 = e^{-1} e^{\mu/kT} e^{-\frac{1}{kT}\gamma\rho_2(1 - a\rho)} \int_{p_0}^{\infty} e^{-p^2/2m\,kT} \frac{d^3p}{(2\pi)^3} \tag{12}$$

and

$$\rho_1 + \rho_2 = \rho, \text{ the density of the total system.} \tag{13}$$

Equation (1) can be written as

$$P = kT\left[\frac{N}{V} - \frac{1}{2}\frac{C}{kT}\left(\left(\frac{N}{V}\right)^2 - a\left(\frac{N}{V}\right)^3\right)\right] \tag{14}$$

and

$$C = \alpha \rho_1^2 + \beta' \rho_1 \bar{\rho}_1 - \gamma \rho_2^2 . \tag{15}$$

From the definition of ρ_1, ρ_2, $\bar{\rho}_1$ and C, the equation of state is that of the ideal gas plus some correction term. Since a N/V is always less than 1, C essentially determines the p - V curve. And α, β', γ are of the same order of magnitude, although they would vary from substance to substance. k_0 most likely is strongly density-dependent, although we must go beyond the Hartree approximation to assess how it depends on the density. From (13), (14), and (15) the sign of C is decided by whether there are more high-momentum particles ($k > k_0$) than low-momentum particles ($k < k_0$), or whether $\rho_1 \gg \rho_2$ and vice versa. It is an inevitable feature of using separable potentials that C depends on the momentum of the individual particles rather than on the relative momentum.

We may have a qualitative discussion of the solutions as follows. With <u>density fixed</u>, when T increases, one can see from (10), (11), (12) and (13) that ρ_1 decreases, and since $\rho_1 + \rho_2 = \rho$, ρ_2 becomes more important. It means high-momentum particles increase in number, a natural consequence of increasing temperature.

Similarly, with the temperature constant, when ρ increases, ρ_1 increases, but not as fast as ρ_2. Although α, β' and γ are not well known numbers, effective mass usually does not increase very fast and is always finite. It seems when ρ is very large, ρ_1 will be "saturated" and ρ_2 will increase without limit.

Let us consider the P - V curve from Eqs. (14) and (15) for a given value of ρ. It is just a cubic equation of ρ,

$$\left\{\left(\frac{V}{N}\right)^3 - \frac{kT}{P}\left(\frac{V}{N}\right)^2\right\} + \frac{kT}{2}\ C\ \frac{V}{N} - a \equiv \left[+ f_1\right] + f_2 = 0 . \qquad (16)$$

It always has one root greater than zero.

From the curve for $\left[f_1\right]$, $\left[f_2\right]$, one sees the solution V is greater than or less than $V_0 = \frac{kT}{\rho}$ (ideal case), depending on whether C is greater than or less than zero.

According to the previous discussion, e is negative when the density is high, and vice versa. This is just what Ref. 4 means by the change from "essentially attractive" to "repulsive" when the density becomes high.

So far we are discussing the limiting case of very high and very low density. The equation for existence of these real roots for Eq. (16) is

$$-\left(\frac{kT}{\rho}\right)^4\left(\frac{c^2}{16.27}-\frac{4ac}{27}\right)+\left(\frac{kT}{\rho}\right)^3\left(\frac{c^3}{27.8}-\frac{ac^2}{3}\right)+\left(\frac{kT}{\rho}\right)^2\frac{c^2a^2}{4} < 0 .$$

Actually, since b and c are both small quantities, it is clear that in (6) there are not three solutions for large P/kT or small values of $\frac{N}{V}$. This indicates that the equation of P - V is really a curve of Van der Waal's type.

One of the most important questions is the validity of the entire approximation, namely, whether $\delta^2 F$ is positive or not. It is not hard to see from general discussions or from general discussions or from the nature of cubic equation (14) that the solution is stable. For the region where three solutions exist, it is hard to discuss analytically, but then we can use Fig. 1 directly.

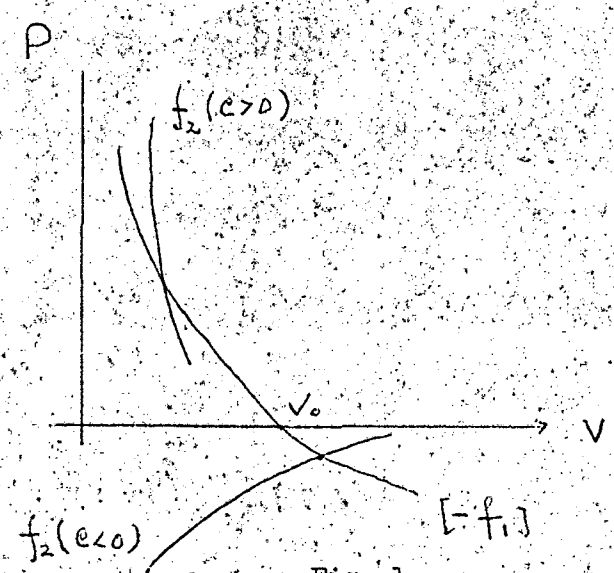


Fig. 1

There are two solutions which satisfy $-\left(\frac{\partial P}{\partial V}\right) > 0$, but when two stable solutions exist, the only one that should survive is the one that makes F relatively smaller. This means that because of the structure of the system, the gas system at certain T and pressure must undergo a dynamical change to form a liquid, so that the volume of the system is changed in such a way that F assumes the smallest possible value.

B. The Ising Model in the Variational Method

The Hamiltonian in which we are interested is

$$H = -J \sum_i \sigma_{i,z}\, \sigma_{i+1,z} - \sum_i \mu H\, \sigma_{i,z} ,$$

where J is positive or negative depending on whether it is a ferromagnetic or an antiferromagnetic system. The trial density matrix is taken as the product of "quasi-particle" density matrices. As will be explained, the different "simple-particle" pictures lead to different answers. We will try to show below how one picture has more advantages than the others.

If the "quasi particles" here are "individual" particles in the lattice, then

$$\rho = \prod_i \rho_i = \prod_i \begin{pmatrix} |a_i|^2 & 0 \\ 0 & |b_i|^2 \end{pmatrix}$$

is in the spin-coordinate system and $|a_i|^2$ means the probability of spin up, $|b_i|^2$ the spin down. We have

$$\mathrm{Tr}\, \rho_i = 1,$$

thus

$$a_i^2 + b_i^2 = 1 .$$

The entropy is

$$-s = k \sum_i \left\{ |a_i|^2 \ \ell n \ |a_i|^2 + |b_i|^2 \ \ell n \ |b_i|^2 \right\}$$

and

$$E = \mathrm{Tr} \ \rho H = -J \sum_i (|a_i|^2 - |b_i|^2)(|a_{i+1}|^2 - |b_{i+1}|^2)$$

$$-\mu H \sum_i |a_i|^2 - |b_i|^2 \ .$$

Let

$$|a_i|^2 = R_i \ .$$

Using the equation $\delta\left(-s + \frac{E}{T}\right) = 0$ and choosing the coefficient of δR_i to be zero, we have

$$\delta\left\{\frac{1}{2} kT(1 + R_i) \ \ell n \ (1 + R_i) + \frac{1}{2} kT(1 - R_i) \ \ell n(1 - R_i)\right\}$$

$$-\delta\left\{J \sum R_i \ R_{i+1} - \mu H R_i\right\} = 0,$$

$$\frac{kT}{2} \ \ell n\left(\frac{1 + R_i}{1 - R_i}\right) - J(R_{i-1} + R_{i+1}) - \mu H = 0 \ , \ i = 0 \cdots N \ .$$

If we take $R_i = R$,

$$R = \tanh 2 \frac{\mu H + 2JR}{kT} \ . \qquad (17)$$

We then have the well-known Bragg-Williams' solution.[11]

The stability of this solution, i.e., $\frac{\delta^2 F}{\delta R} > 0$, is discussed in books on statistical mechanics.[11] We know this solution is far from the exact one of the one-dimensional Ising model,[12] but the curve of the specific heat obtained from this solution resembles the experimental curve. Perhaps this indicates that our Hartree approximation is good only for the long-range force, i.e., the more interaction particles with range of the force, the better. As a matter of fact, it has been shown that the one-dimensional Ising model with infinite long-range force will have the Bragg-Williams' solution. The success of the theory of high-density electron gas, using the random phase approximation, is another good example.

As has been emphasized, quasi particles are not well defined; different quasi particles will be used to examine which is better. We may also use wave-type quasi particles, for instance: expand R_n as

$$R_n = \frac{1}{N} \sum_{k=0}^{\infty} e^{inka/N} R(k) \tag{18}$$

where a is the interparticle distance, N the number of particles. In Heisenberg's theory of ferromagnetism, $R(k)$ will be a spin-wave operator, and our variational principle can be used to obtain the results of the spin-wave theory in a similar fashion. Certainly this result is not surprising, since it is only the Hartree-Fock

approximation.

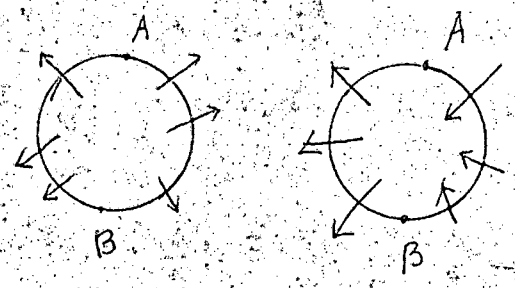
If expansion (18) is made in the Ising model we will obtain $R(k) = \tanh 2\left[\frac{\mu H+2JR(k)}{kT}\cos\frac{ka}{N}\right]$ and this answer is better than the one given in (17), since it yields a lower free energy, but does not change the essential features.

In our approximation, correlation of particles has been neglected completely, and this is the primary reason why there is a phase transition in two dimension, but not in one dimension, as R. E. Peierls has pointed out. Therefore, we do not expect any reasonably close answer to the exact solution in our approximation.

It has been emphasized that the power of the variational principle is that we have the freedom to use the most appropriate quasi particle.

Our previous approximation is not valid for the Ising model, but we can improve it by taking different quasi particles. Let us specify the states by the number of foreign neighbors in the one-dimensional problem. (We count one foreign neighbor as one consecutive pair with one spin up and one spin down.) Denote this state by f_k^n, with n the number of spins up, $2k$ the number of foreign neighbors. The contribution of one configuration to the entropy is $-\frac{1}{\beta} f_{2k}^n \ln f_{2k}^n$. It would be wrong to put the total entropy to be the summation over k, and n, since there are 2^N possible configurations; each configuration does not have the same weight. The energy of this configuration is $-J(N-4k)f_k^n$

(there are 2k foreign neighbors in the configuration) which is independent of n in the absence of magnetic field. In the one-dimensional problem we always can pick 2k lattices among N particles to form 2k pairs of foreign neighbors. For instance, in the picture we pick A, B as two arbitrary points and change the directions of spins between A and B.



This process can be continued, and has nothing to do with the original orientational spins.

Furthermore,

$$\sum_{k=0}^{N/2} C^N_{2K} = 2^N,$$

thus

$$\text{total energy} = -J \sum_k C^N_k (N - 2k) f_k ,$$

$$\text{total entropy} = -(\beta T)^{-1} \sum_k C^N_k f_k \ln f_k ;$$

$$\delta F = 0 \text{ implies } f_k = e e^{-\beta T(N - 2k)} ,$$

$$e^{-F/kT} = \sum_{k=0}^{N/2} C^n_k e^{-\beta J(N-2k)} = \left(e^{J/kT} + e^{-J/kT}\right)^N$$

$$= \left(2 \cosh J/kT\right)^N .$$

This is the exact answer of the one-dimensional Ising model. Since it is simple to obtain, it seems useless to do it our way, but our purpose is only to illustrate the idea of using the variational principle.

Our method is hard to extend to the two-dimensional problem. Some early works on the Ising model engaged in the "counting" of all possible configurations ran into the same problem. Since it has been reviewed intensively, we do not repeat it here.

C. Statistical Mechanics of He^4 Above the Transition Temperature

The specific heat of He^4 has been recently calculated,[14] by use of the Hartree-Fock approximation. The pseudo-potential approximation is used for the hard core, and

$$\langle k|V_{\text{attractive part}}|k\rangle = \alpha + \beta k^2$$

is assumed.

As $V_{\text{attractive}}$ is finite and converges fast enough for large distances, α and β are defined. (The 6-12 potential is used in Ref. 14.) The total potential is $\alpha + \beta k^2 + a$ (a is the radius of the hard core).

Above the transition temperature the result of this calculation gives a specific heat five times as high as the experimental values, but there are two questionable points in Ref. 14. First, the calculation is thermodynamically inconsistent: the total energy is not the same as given by $\frac{\partial F}{\partial \beta}$; here F = free energy, $\beta = (kT)^{-1}$. It is hard to see why one has to use $\frac{\partial F}{\partial \beta}$ for total energy. Another question is that to use the Hartree-Fock approximation, it is necessary to examine whether the solution is thermodynamically stable.

The potential with a hard core does not have a Fourier transform, the only more or less satisfactory way to do the calculation is to put

$$\langle k|V|k\rangle = \langle k|T_0|k\rangle = -\frac{4\pi}{m}\frac{1}{k}\sin\delta\cos\delta ,$$

where δ is the phase shift of two free particles. This means that the potential between two particles is replaced by the effective interaction $\langle k|T_0|k\rangle$, which is the summation of the ladder diagrams with the free-particle propagator, and furthermore is density independent.

A rigorous T approximation means the summation of the ladder diagrams with real quasi-particle propagator, and this exact T, in principle, can be expanded in terms of powers in T_0 and is strongly density dependent. If we take the first order of T_0 as the interaction, then we have for the entropy S, energy E, and free energy F

$$TS = \beta^{-1}\left[\rho_k \ln \rho_k - (1 + \rho_k) \ln(1 + \rho_k)\right] ,$$

$$E = \sum_k k^2/2m \; \rho_k + \frac{1}{2} \; \rho_{k_1} \left\langle \frac{k_1 - k_2}{2} \middle| T_0 \middle| \frac{k_1 - k_2}{2} \right\rangle \rho_{k_2} ,$$

$$F = E - TS - \mu N .$$

Here ρ_k is the distribution of the quasi particle of momentum k:

$$\frac{\delta F}{\delta \rho_k} = 0 ;$$

ρ_k is thus determined to be

$$\frac{1}{\exp\left\{\beta\left[k^2/2m + \sum_{k_2} \rho_{k_2} \left\langle \frac{k - k_2}{2} \middle| T_0 \middle| \frac{k - k_2}{2} \right\rangle - \mu\right]\right\} - 1} .$$

$\frac{\delta^2 F}{\delta\rho_k \, \delta\rho_{k'}}$ has to be discussed, and it is

$$\beta^{-1} \sum_k \delta\rho_k \frac{1}{\rho_k} \frac{1}{1+\rho_k} \delta\rho_k + \sum_{kk'} \delta\rho_k \left\langle \frac{k-k'}{2} \middle| T_0 \middle| \frac{k-k'}{2} \right\rangle \delta\rho_{k'} . \tag{19}$$

To discuss whether (19) is positive or negative is very hard, but we are interested only in the region where the temperature is very close to the transition temperature. The ρ_k may be written as

$$\left[\exp\left[\beta(k^2/2m^* - \mu') + \text{higher power in } k^2\right] - 1\right]^{-1} ,$$

and $\mu' \to 0$ when $T \to T_\lambda$; ρ_k will be large for small k .

Equation (19) is a quadratic. It will be positive definite if $\delta^2 F/\delta\rho_k \delta\rho_k$ has no negative eignevalue. We take only the diagonal term $k \approx 0$, $k' \approx 0$, which is the dominating term when $T \to T_\lambda$. Expand (19) , and when μ/kT is small it reduces to

$$kT\left(\frac{\mu'}{kT}\right)^2\left(1 + \frac{\mu'}{kT}\right) + \frac{N}{V} \langle 0|T_0|0\rangle . \tag{20}$$

Here N actually is the number of particles with momentum zero, or

approximately the number of particles in the system interacting with $\langle 0|T_0|0\rangle$, and this should be about the order of N.

The following numbers are taken from Ref. 15 and 16.

Temperature	Density (g/cm^3)	μ/kT
2.2	0.146	0
3.0	0.141	$\approx 10^{-3}$
4.0	0.128	$\approx 10^{-2}$

If we believe that the first order of T_0 is going to give us a reasonable answer, T_0 must be negative, since it is proportional (roughly) to the ground-state energy. Thus, $\mu \to 0$ when $T \to T_\lambda$; (20) must be negative. This means that the solution given by the first order of T_0 cannot give us a sensible solution to guarantee $\delta^2/\delta\rho\delta\rho$ is positive.

Our arguments are not rigorous at all, but they show that simple calculations cannot provide meaningful answers. The simplest extension is to attempt a better solution for T in Eq. (21).

$$\langle k|T|k'\rangle = \langle k|V|k'\rangle + \int \frac{\langle k|T|k''\rangle\{s.f.\}\ \langle k''|V|k'\rangle}{k^2/2m - k''^2/2m + \Sigma(k_1) + \Sigma(k_2) - \Sigma(k_1'') - \Sigma(k_2'')} \times \frac{d^3k'}{(2\pi)^3}, \qquad (21)$$

where s.f. = statistical factor.

$$\text{s.f.} = \coth \frac{1}{2} \frac{\omega_1'' - \mu}{kT} + \coth \frac{1}{2} \frac{\omega_2'' - \mu}{kT} ,$$

$$\omega_1'' = \frac{k_1''^2}{2m} + \Sigma(k_1'') .$$

Here Σ is the self-energy of the particle in the medium; s.f. $\rightarrow 1$ only for $\mu = 0$, $kT \rightarrow 0$ for k_1'' and k_2'' not zero. Therefore, the exact T equation is too far away from T_0, which satisfies

$$\langle k|T_0|k'\rangle = \langle k|V|k'\rangle + \int \frac{\langle k|V|k''\rangle\langle k''|T_0|k'\rangle}{k^2/2m - k''^2/2m} \frac{d^3k''}{(2\pi)^3} .$$

The expansion of T in terms of T_0 as mentioned in the next part should be interesting, since the complicated dependence of T on temperature might reveal the behavior of the specific heat of He^4. We realize that Eq. (21) is still an approximation in the quasi-particle picture, but it is believed that above the transition temperature, it is the statistical factor that plays an important role and the quasi particle used should be reasonably justified. We may also use a simple potential and calculate $\langle k|T_0|k'\rangle$ easily just to see how the statistical factor influences the results.

With these approximations, it seems, at least, we can justify our calculation; namely, our solution will be thermodynamically stable. In simple effective mass approximations, $\langle 0|T_0|0\rangle$ will

be positive if input and output m^* are consistently calculated. As a matter of fact, we can obtain the transition temperature from this effective mass approximation, and thermodynamically it is a stable solution, but to obtain the specific heat is not simple.

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* This work done under the auspices of the U. S. Atomic Energy Commission.

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I. INTRODUCTION

We wish to present a way of calculating equilibrium properties of a fermion system with high density and strong short-range force but relatively weak long-range force. He^3 serves as an example. As far as the theory is concerned, it has been discussed repeatedly.[1-3] We will use the thermodynamical Green's function,[4,5] and the T approximation, which is essentially the Brueckner's reaction matrix method.

The validity of the T approximation is well understood, namely it is a good approximation for low density and short-range force.[5] Some arguments have been given that because of the strong degeneracy of the fermion system, interactions take place only among the particles at the Fermi surface. The success of Landau's theory seems to justify this assertion.

There is no reason to believe that an approximation which involves more than two-body correlation will not substantially change the results in a system like He^3. It should also be pointed out that rigorous treatment of the T approximation in the Green's-function formalism is more complicated than calculations done in Ref. 1. As a simple example, we will see that the imaginary part of the self-energy is fairly large, which indicates that the spectral function is far from a delta function, and a complicated renormalization factor must be used, though how much it influences the results is not known.

It is not our intention here to solve this problem, rather we wish to do a calculation similar to that of Ref. 1 in a slightly different formalism. The purpose is to calculate the diagonal T-matrix elements (the forward scattering amplitude of two quasi particles in the medium).

In Ref. 1, the integral equation for the reactionmatrix is set up and the single-particle energy is obtained consistently. It is very difficult to solve the integral equation involving the principal part.[6] It is hoped that this can be avoided and a differential equation will emerge instead. In order to accomplish this purpose, there are two simplifications to be made:

(a) The statistical factor in the intermediate states will be ignored,

(b) the single-particles energy will be taken to be of the form $A + BK^2$.

The correction due to the hole-hole term is believed to be small, though this contribution is of higher power in density, and the density of liquid He^3 is high. However, it will be shown that to neglect the statistical factor at first in the calculation of t and then to make a correction later is justifiable, considering the other approximations we have to make. We write the single-particle energy $\omega(p) = A + B\,p^2/2$, where B^{-1} will mean effective mass of the He^3 and A will not appear in the T equation. There is no compelling reason to say

that this approximation is good, only experience can tell. Under these assumptions, the T equation will become the free-particle scattering equation with mass $\frac{1}{B}$, which can be readily solved.

There has been some argument about the boundary condition in the reaction matrix, i.e., whether the two-particle wave function should be outgoing or stationary.[7]

In principle, this has been answered[8] after careful study of the limiting process as the volume $\rightarrow \infty$, but it seems doubtful that the arguments are still valid for a strongly interacting system at high density. The diagonal terms of T are related to the phase shifts by solving the Schrödinger equation with different boundary conditions: $\langle k|T|k\rangle = -\frac{4\pi}{mk} \tan \delta$, if the principal part is taken, or $\langle k|T|k\rangle = -\frac{4\pi}{mk} e^{i\delta} \sin \delta$, for the outgoing condition. In Green's-function formalism this problem (the boundary condition) is settled from the beginning.

Instead of effective mass approximation, calculations similar to Ref. 3 can also be used in He^3, but certainly it is not correct in He^3 to consider the attractive part as "small."

Section II is a brief summary of the formalism of thermodynamical Green's functions. We treat fermions and bosons all together at first. Since the formalism has been intensively discussed in the literature, we give only the relevant equations which are necessary to explain the calculation.

In Section III the T approximation is used to obtain the

effective mass, with the assumption that the single-particle energy is written as $A + k^2/2m^*$. Calculations of velocity of sound are discussed, and show the strong density dependence of the T matrix.

Sections IV and V deal with the correction due to the exclusion principle in the intermediate states and calculation of the ground-state energy.

II. THEORY OF GREEN'S-FUNCTION FORMALISM

The general theory has been given many times in the literature and summarized in Ref. 5. We will only present the necessary formulae for convenience and reference.

Let us denote ψ^+, ϕ^+ as creation operators of He^3, He^4 respectively. The total Hamiltonian is

$$
\begin{aligned}
H = & \frac{1}{2m}\int \nabla \psi^+ \cdot \nabla\psi + \frac{1}{2m'}\int \nabla \phi^+ \cdot \nabla \phi \\
& + \frac{1}{2}\int \psi^+(r_2)\, \psi^+(r_1)\, V(r_1-r_2)\, \psi(r_1)\, \psi(r_2)\, d^3r\, d^3r_2 \\
& + \frac{1}{2}\int \phi^+(r_2)\, \phi(V_1)\, V'(r_1-r_2)\phi(r_1)\phi(r_2)\, d^3r_1 d^3r_2 \\
& + \int \psi(r_1)\, \phi(r_2)\, V_{12}(r_1-r_2)\, \psi(r_1)\, \phi(r_2)\, d^3r_1 d^3r_2 \, .
\end{aligned}
\tag{1}
$$

V means the potential between particles and ψ, ϕ obey the usual anticommutation and commutation rules. Let

$$G(11') = \frac{1}{i}\, T\langle \psi(1)\, \psi^+(1')\rangle \, ;$$

then

$$G^{>}(11') = \frac{1}{i}\, \langle \psi(1)\, \psi^+(1')\rangle \qquad \text{if } t_1' > t_1 \, ,$$

and

$$G^{<}(11') = -\frac{1}{i}\, \langle \psi^+(1')\psi(1)\rangle \qquad \text{if } t_1 > t_1' \, .$$

Similarly we define

$$g(11') = \frac{1}{i} T\langle \phi(1)\, \phi^{+}(1')\rangle \quad .$$

We also define $G_2(12, 1'2')$ and $g_2(12, 1'2')$, the two-particle Green's functions of He^3 and He^4, respectively, as they are defined in Ref. 1. Here $G'(12, 1'2')$ is the Green's function for ϕ and ψ, namely,

$$G'(12, 1'2') = T(\psi(1)\, \phi(2)\, \psi^{+}(1')\, \phi^{+}(2')).$$

The equations of motion are

$$\left(i \frac{\partial}{\partial t} + \frac{\nabla_1^2}{2m} - \mu\right) G(11') = \delta(11') - i \int v(r_1 - r_2)\, G_2(12, 1'2') \Big|_{t_2 \to t_2'} d^3 r_2$$

$$+ i \int v_{12}(r_1 - r_2)\, G'(12, 1'2') \Big|_{t_2 \to t_2'} d^3 r_2 \quad . \tag{2}$$

The equations for $g(11')$, and $G'(11')$ are similar. Using the T approximation, which is discussed in Refs. 4 and 5, we have

$$G_2(12, 1'2') = G(11')\, G(22') - G(12')\, G(21')$$

$$+ i \int_0^{-i\beta} d\bar{1}\, d\bar{2}\, G(1\bar{1})\, G(2\bar{2})\, V_1(\bar{1}\,\bar{2})\, G_2(\bar{1}\,\bar{2}, 1'2') \; . \tag{3}$$

Since $G_2'(12, 1'2')$ and $g(12, 1'2')$ are so similar to G_2, we will not write them down here.

The approximation in terms of diagrams means that all ladder diagrams with an exact Green's function in the intermediate state are taken in calculation of the ground-state energy. For instance, G_2, g_2, G_2', defined as above can be expressed in terms of the T matrix,

$$G_2(12, 1'2')V(1'2') = \int \langle 12|T|\bar{1}\,\bar{2}\rangle\, G(\bar{1}, \bar{1}')\, G(\bar{2}, \bar{2}')\, d^3\bar{1}\, d^3\bar{2}\,, \tag{4}$$

where T is defined as

$$\langle 12|T|1'2'\rangle = V(12)\,\delta(11')\,\delta(22') + i\int_0^{-i\beta} d\bar{1}\, d\bar{2}\, \langle 12|T|\bar{1}\,\bar{2}\rangle\, G(\bar{1}, 1')\, G(\bar{2}, 2')\,. \tag{5}$$

Similarly we can define t for g_2, and T' for G_2'.

Using (4) and (5) (1) and (2) become

$$\left[i\frac{\partial}{\partial t} + \frac{\nabla_1^2}{2m} - \mu\right] G(11') = \delta(11') + \int_0^{-i\beta} \sum_{\sigma} (1\bar{1})\, G(\bar{1}\, 1')\, d^3\bar{1} \tag{6}$$

and

$$\Sigma = \int \left[\langle 12|T|1'2'\rangle - \langle 12|T|\bar{2}\,\bar{1}\rangle\right] G(2, \bar{2})\, d\bar{1}\, d\bar{z}$$

$$+ \int \langle 12|T'|\bar{1}\,\bar{2}\rangle\, g(\bar{2}\, 2^{+})\, d\bar{1}\, d\bar{z} \,. \qquad (6a)$$

Here T' is the scattering amplitude between He^3 and He^4. $g'(11')$ is similar to this. He^3, He^4 are different types of particles, thus we do not have an exchange term for T'.

Due to the periodicity of the thermodynamical Green's function, we can expand $G(11')$ and T in Fourier series. For instance,

$$\langle 12|T(t_1-t_1')|1'2'\rangle = \frac{1}{-i\beta} \sum_{\nu} e^{-Z\nu(t_1-t_1')} \langle 12|T(Z\nu)|1'2'\rangle \,,$$

$$Z\nu = \pi\nu/-i\beta + 2\mu \,, \text{ where}$$

where ν are even integers. Similarly,

$$G(t_1-t_1') = \frac{1}{-i\beta} \sum e^{-Z\nu(t_1-t_1')}\, G(Z\nu) \,,$$

$$Z\nu = \frac{\pi\nu}{-i\beta} + \mu \,,$$

where ν are odd integers. Furthermore we take the Fourier integral of Eqs. (2) and (3):

$$\left(i\frac{\partial}{\partial t} - k_1^2/2m - \mu\right) G(k_1, t_1 - t_1') = \delta(t - t')$$

$$+ i\int d^3k_2\, dt''\ \langle k|T(\bar{p}, t_1 - t_1'')|k\rangle\, G(k_2, t_1'' - t_1') \cdot G(k_1, t_1'' - t_1')$$

$$+ \text{term due to } He^3 - He^4 \text{ scattering.} \qquad (7)$$

Here we have defined the Fourier transform for a four-point space function as follows:

$$\langle p|T(\bar{p}, z)|p'\rangle = \int \frac{d^3(\underset{\sim}{r}_1 - \underset{\sim}{r}_2)}{(2\pi)^3} \int \frac{d^3(\underset{\sim}{r}_1' - \underset{\sim}{r}_2')}{(2\pi)^3} \int \frac{d(\underset{\sim}{p} - \underset{\sim}{p}')}{(2\pi)^3}$$

$$\times e^{-i\underset{\sim}{p}(\underset{\sim}{R} - \underset{\sim}{R}')}\, e^{i(\underset{\sim}{r}_1 - \underset{\sim}{r}_2)\cdot p}\, e^{-i\,\underset{\sim}{p}(\underset{\sim}{r}_1' - \underset{\sim}{r}_2')} \langle r_1 r_2|T(z)|r_1' - r_2'\rangle .$$

Here $\bar{p}$, p, p' mean momentum of the center of mass, and relative momenta of the two particles, respectively.

After expressing G_1, G_2 and T in terms of their Fourier coefficients, Eqs. (6) and (7) become

$$\left[\frac{\Pi\nu}{-i\beta} + \mu - \frac{k_1^2}{2m} - \Sigma_1(k_1\ \nu) - \Sigma_2(k_1\ \nu)\right] G(k_1\ \nu) = 1 .$$

The details are given in Appendix I. Σ_1 is the contribution from $He^3 - He^3$ scattering, and Σ_2 comes from the contribution of $He^3 - He^4$ scattering, and Σ_2 will be neglected from now on:

$$\Sigma_1(k_1\ \nu) = \sum_{\nu'} \int G(k_2,\ \nu)\ \langle k|T(\bar{p},\ \nu + \nu')|k\rangle\ \frac{1}{-i\beta}\ \frac{d^3k_2}{(2\pi)^3}. \quad (8)$$

The details are given in the Appendix. One has to solve Eqs. (5), (6) and (8) consistently to obtain the T approximation. It is exceedingly difficult to obtain a spectral function defined by

$$G(k,\ \nu) = \frac{1}{2\pi}\int d\omega\ \frac{A(k,\ \omega)}{\omega - \nu}\ .$$

In Brueckner's calculation $A(k,\omega)$ is implicitly taken to be $2\pi\ \delta(\omega - \omega(k))$, and $\omega(k)$ is determined self-consistently. We will take $A(k,\omega)$ as a delta function also. It is noted. however, from a general theorem,[9] proved in a perturbation expansion, that

$$A(k,\ \omega) = Z_k\ \delta\left[\omega - \omega(k)\right]$$

when $k \to k_f$, though we cannot justify our approximation by

proving Z_k is about 1.

There are two other major differences between the T equation given in Ref. 5 and Brueckner's integral equation for the reaction matrix, G is the propagator of two particles in the medium. The principal part is taken somewhat arbitrarily and a singularity will be expected. This problem is settled for a system of low density and weak interaction in Ref. 8--namely, as follows: the diagonal matrix element of the R matrix is proportional to tan δ, where δ is the phase shifts of two bare particles. If the level shift of the single-particle energy in the medium is introduced, R defined by the integral equation is proportional to δ instead of tan δ. However, with a very strong force and high-density system, such as He^3, the problem is hard to answer, but the Green's function formalism does provide the boundary condition unequivocally in the T matrix.

After the spectral function is taken to be a delta function, the T matrix defined in Eq. (5) is

$$\langle p|T(p, z)|p'\rangle = \langle p|v|p'\rangle + \int \frac{d^3\bar{p}_1\, d^3\bar{p}_2}{(2\pi)^b} \langle p|T(\bar{p}, z)|\bar{p}\rangle\langle\bar{p}|v|p'\rangle g(\bar{p}_1, \bar{p}_2) . \tag{9}$$

Here g means the product of two one-particle Green's functions in the intermediate state with momenta and energies $\bar{p}_1$, $\bar{p}_2$, $\bar{\omega}_1$, $\bar{\omega}_2$.

More explicitly,

$$g = \frac{f(\bar{p}_1)\, f(\bar{p}_2) - (1 - f(\bar{p}_1))(1 - f(\bar{p}_2))}{z - \bar{\omega}_1 - \bar{\omega}_2}, \qquad (10)$$

where f is the Fermi distribution, and z is the total energy of two particles.

This equation is exactly the same as Brueckner's equation except that $\langle p|T(z)|p'\rangle$ for real z is taken to be $\lim_{\epsilon\to 0} \langle p|T(z + i\epsilon)|p'\rangle$. To solve even this equation is an exceedingly complicated computation.[7] In the following we proceed to make an approximate calculation, in which an integral equation is reduced to a differential equation. After some approximations have been made, Eqs. (9) and (10) are still far from being easily solved. The fairly general equation for the T matrix would be

$$\langle p|T(z)|p'\rangle = \langle p|v|p'\rangle + \int \langle p|v|p''\rangle \frac{f(p_1'', p_2'')}{z-\omega_1''(p_1)-\omega''(p_2)} \langle p''|T|p'\rangle \frac{d^3p''}{(2\pi)^3}. \qquad (11)$$

(Contributions from the cut discussed in Appendix I is still neglected here, but it is not too relevant to our discussion.

To solve (11) by expansion in terms of $\langle p|v|p'\rangle$ is simply impossible, actually $\langle p|V|p'\rangle$ does not exist in our case, but we may expand $\langle p|T|p'\rangle$ in terms of a quantity which will be convergent rapidly as follows.

The only soluble integral equation of Type (11) is

$$\langle p|T_0|p'\rangle = \langle p|v|p'\rangle + \int \langle p|v|p''\rangle \frac{1}{\left(p^2/2m\right) - \left(p''^2/2m\right) + i\epsilon} \langle p''|T_0|p'\rangle \frac{d^3p''}{(2\pi)^3} \tag{11'}$$

and

$$\langle p|T_0|p\rangle = -\frac{4\pi}{mp} \sin\delta(p)\, e^{i\delta(p)} ,$$

the phase shifts calculated from solving the Schrödinger equation. Then (11) can be expressed in terms of $\langle p|T_0|p\rangle$ as follows:

$$\langle p|T|p'\rangle = \langle p|T_0|p'\rangle + \int \langle p|T_0|p''\rangle \times \left\{ \frac{f(\omega_1'' \; p_2'')}{z-\omega_1''-\omega_2''} - \frac{1}{\left(p^2/2m\right) - \left(p''^2/2m\right)} \right\} \langle p|T|p'\rangle \frac{d^3p''}{(2\pi)^3} \times \left\{ \frac{f(\omega'' \; ; p_2'')}{z-\omega_1''-\omega_2''} - \frac{1}{\left(p^2/2m\right) - \left(p''^2/2m\right)} \right\} \langle p|T|p'\rangle \frac{d^3p''}{(2\pi)^3} . \tag{12}$$

When $\langle p|T_0|p'\rangle$ is expressed in terms of phase shifts, the expansion of (12) in terms of $\langle p|T_0|p'\rangle$ makes sense. At least, it is much better than to expand T with potential, but one must have the off-diagonal elements $\langle p|T_0|p'\rangle$, with $p \neq p'$, to do the calculation. It seems that the only reasonable and simple way to do the calculation is to use some simplified potential which fits the phase shifts well and to solve the Schrödinger equation with that potential. Actually Ref. 10 is one example. Perhaps one can use some separable potential

$$\langle p|v|p'\rangle = v_1(p)\, v_1(p')$$

to fit the phase shifts and make the complete solution of (12) possible. It has been found, however, that there is no unique choice of a separable potential, and different separable potentials which yield the same phase shifts will make off-diagonal elements of the T matrix entirely different.[6]

Equation (12) is still too difficult to solve, but it certainly is useful to investigate how large some neglected effects are, for instance, the magnitude of the renormalization constant and the effect of the exclusion principle in the intermediate states, which will be approximately estimated in later sections from (12).

Since only (11') can be solved through the Schrödinger equation, we expand

$$\omega - \mu = \frac{k^2}{2m} + \Sigma(k, \omega) = \frac{1}{2m^*}(k^2 - k_f^2) ,$$

$\Sigma(k,\omega)$ is taken to be $\Sigma(k_f) + \frac{\partial\Sigma}{\partial k^2}(k^2 - k_f^2)$, and $\frac{\partial\Sigma}{\partial\omega}$ is neglected here. It measures the width of the spectral function, or the deviation from our assumption that the spectral function is a delta function. We have

$$\frac{1}{m^*} = \lim_{k \to k_f} \frac{\partial\Sigma}{\partial k^2} . \tag{13}$$

After the imaginary part of T, which is proportional to T_0^2, is neglected in (9) and (10), and $\frac{\partial\Sigma}{\partial\omega}$ is regarded as small which is also of order T_0^2. With all these approximation, we have to solve (9) and (10):

$$\langle p|T_0|p'\rangle = \langle p|v|p'\rangle + \int \frac{d^3p''}{(2\pi)^3} \frac{\langle p|v|p''\rangle \, Q \, \langle p''|T_0|p'\rangle}{\left(p^2/2m^*\right) - \left(p''^2/2m^*\right)} ,$$

where

$$Q = 1, \text{ if } p_1'', \text{ and } p_2'' \geqslant p_F ,$$
$$Q = -1, \text{ if } p_1'', \text{ and } p_2'' \leqslant p_F .$$

Correction to the approximation that Q is taken to be 1, which

will be made later on, is also of order T_0^2. The difficult point in high-density systems is that higher powers in T_0 are not necessarily small. Even in higher angular momenta, because of the factor $(2\ell + 1)$, the contribution is not small.

In the following calculation, we solve only for T_0 and use it throughout the whole work; it will be seen that the correction is not always small enough to be neglected. Perhaps it is necessary to solve (12) roughly to see the order of magnitude of the correction to T.

III. CALCULATION OF EFFECTIVE MASS AND SOUND VELOCITY IN He^3

From the expression for m^* in (13) and Eqs. (8) and (A.4), we have

$$\frac{1}{m^*} = \frac{1}{m} + \lim_{p_1 \to p_F} \frac{1}{p_1} \frac{\partial}{\partial p_1} \int \langle p|T_0|p\rangle \left(\frac{1}{e^{(p_2^2 - p_F^2)/2m^*kT} - 1} \right) \frac{d^3p_2}{(2\pi)^3} ; \tag{14}$$

thus

$$\frac{1}{m^*} = \frac{1}{m} + \int \langle p|T_0|p\rangle \; \delta(p_2 - p_F) \frac{2\pi \, p_2^2 \, dp_2}{(2\pi)^3} \cos\theta \, d\cos\theta .$$

Expand $\langle p|T_0|p'\rangle$ in angular momentum states:

$$\langle p|T_0|p'\rangle = \sum_{\ell,m} \langle p|T_0^{\ell}|p'\rangle \; Y_\ell^m(\cos\theta) \, Y_\ell^m(\cos\theta') ,$$

and

$$\langle p|T_0^{\ell}|p'\rangle = -\frac{4\pi}{m^*} \frac{1}{p} e^{i\delta_\ell} \sin\delta_\ell ;$$

P is the relative momentum $= \frac{1}{2} |p_1 - p_2|^{\frac{1}{2}} = p_F \sin(\theta/2)$, if $|p_1| = |p_2| = p_F$. Thus

$$\frac{1}{m^*} = \frac{1}{m} + \frac{2}{\pi} \frac{1}{m^*} \int_0^{\pi} d\theta \frac{\cos\theta \sin\theta}{\sin(\theta/2)} \sum_{\ell} e^{i\delta_\ell} \sin\delta_\ell \begin{Bmatrix} 3(2\ell+1) \text{ for odd } \ell \\ (2\ell+1) \text{ for even } \ell \end{Bmatrix}$$

Here the exchange part is taken equal to the direct part, and only the real part of T is to be integrated. Sin $\delta_\ell(m^*)$ is calculated as described in Section II, the values of different sin $\delta_\ell(m^*)$ are tabulated for the Y - S potential used by Brueckner and the 6 - 12 potential.[12] The results are given as follows for the 6 -12 potential .

Input effective mass	Output m^*
5	4.8
7	9.6

We use Y - S potential from now on. The results for effective mass are as follows:

Input (without correction)	Output mass
6	3.9
7	5.7
8	6.6
8.5	8.4

If we include a correction due to exclusion principle (see Appendix II and Section III), then, if we use phase shifts for $m^* = 7$, the contribution to the output m^* is about 0.6. The number does not vary too much for different input m^* . Since phase shifts are very sensitive to input m^*, it seems that a consistent m^* should be between 7 and 8 .

The numerical values of phase shifts are given in Tables I and II, and plotted in Fig. 1. All these curves are qualitatively

the same as Brueckner's diagonal elements of K^{11}, except for an attractive bump in $\ell = 0$.

There are two questions to be answered:

(a) How does the "rearrangement energy" in Brueckner's theory come in?

(b) What is the relation between our T matrix and Landau's forward scattering amplitude?

"Rearrangement energy" is the correction to $\Sigma(k)$ so that $\Sigma(k) = \frac{\delta E}{\delta f_k}$ (where E is total energy and f_k is Fermi distribution). It is of higher power in T. Since we have neglected T_0^2 in different places, as mentioned before, it would be hardly justified to calculate the correction in Brueckner's way and claim it is the right amount of correction. Thus T_0^2 terms will be neglected here.

Landau's forward scattering amplitude is shown to be $f_{kk'} = \frac{\delta^2 E}{\delta f_k \delta f_{k'}}$ (where E is total energy, f_k is quasi-particle distribution function); $f_{kk'}$ is our T_0, if we approximate the real T as T_0. Thus we see the success of Landau's semi-phenomenological theory is due to the fact that $f_{kk'}$ obtained from experimental m^* and sound velocity includes higher power in T_0. If T_0^2 is neglected throughout the whole calculation, the expression for sound velocity is the same as given in Landau's theory, with $f_{kk'}$ replaced by T_0:

$$c^2 = \frac{p_f^2}{3m^2}\left(1 + \frac{m}{m^*}\frac{2}{\pi}\int_0^\pi \left[\sum_{\ell\ \mathrm{odd}} (2\ell+1) + \sum_{\ell\ \mathrm{even}} 3(2\ell+1)\right] \times \sin\delta_\ell \cos\delta_\ell (1 - \cos\theta)\, d\theta\right).$$

Using our values of δ_ℓ, we obtain $C^2 < 0$. This seems to hold also for Brueckner's results, but a reasonable number will be obtained, if

$$C^2 = \frac{1}{m} N \frac{d\mu}{dN} = \frac{1}{m} N \frac{d^2E}{dN^2}$$

is used. It shows that higher powers in T_0 are of vital importance in the calculation of sound velocity. We mentioned that T_0^2 is small, but $\frac{dT_0}{dN}$, which can be derived from (11'), and is proportional to

$$\int \langle k|T_0|k''\rangle \frac{d^3k''}{(2\pi)^3} \frac{1}{k^2 - k''^2} \langle k''|T_0|k\rangle \frac{dm^*}{dN}$$

and $\frac{dm^*}{dp_F} \frac{p_F}{m^*} = 2.8$, from the experimental data. The strong density dependence of T makes the calculation of the velocity of sound harder than other quantities. We do not mean to go beyond first order in T_0 here; thus a more detailed study of this problem cannot be given.

IV. CORRECTION DUE TO EXCLUSION PRINCIPLE

Our T matrix satisfies the integral equation

$$\langle k|T|k'\rangle = \langle k|v|k'\rangle + \langle k|v|k''\rangle \frac{(Q(k'') - 1)\langle k''|T|k'\rangle}{E - E_1(k'') - E_2(k') + i\epsilon} \frac{d^3k_2''}{(2\pi)^3},$$

where E is the total energy, $Q(k'')$, as was explained before, is

2 when $|k_1''| \geqslant k_F$ and $|k_2''| \geqslant k_F$,

1 when $|k_1''| \geqslant k_F$ and $|k_2''| \leqslant k_F$ (or vice versa),

and 0 when $|k_1''| \leqslant k_F$ and $|k_2''| \leqslant k_F$.

We can express T in terms of T_0 given in (9) by a Heitler type of integral equation.

$$\langle k|T|k'\rangle = \langle k|T_0|k'\rangle + \int \frac{d^3k''}{(2\pi)^3} \langle k|T_0|k''\rangle \frac{Q(k'') - 2}{E - E(k_1'') - E(k_2'') + i\epsilon} \langle k''|T|k'\rangle.$$

If $\langle k|T|k'\rangle$ on the right-hand side is replaced by $\langle k|T_0|k'\rangle$, it means that only the second-order term in the expansion is taken. We do not know how to calculate off-diagonal elements $\langle k|T_0|k'\rangle$ easily. Brueckner does consider them carefully.[10] Here we follow the usual approximation of putting

$$\int \frac{d^3k''}{(2\pi)^3} \left|\langle k|T_0|k''\rangle\right|^2 \frac{Q(k'') - 2}{E - E_1''(k_1'') - E(k_2'') + i\epsilon}$$

$$= \left|\langle k|T_0|k\rangle\right|^2 \int \frac{d^3k''}{(2\pi)^3} \frac{Q(k'') - 2}{E - E(k_1'') - E(k_2'') + i\epsilon} . \quad (15)$$

Therefore the corrected diagonal element is, after partial-wave expansion,

$$\langle k|T_0^{\ell}|k\rangle + \frac{2\pi(2\ell + 1)^2 \left|\langle k|T_\ell^0|k\rangle\right|^2}{(2\pi)^3} \rho \int_{-1}^{1} \rho_\ell^2(\cos\theta) d\cos\theta$$

$$\times \int \frac{k''^2 dk''(Q - 2)}{(k^2 - k''^2)/m^*} . \quad (16)$$

The region of integration is shown in the figure.

where $Q - 2 = -2$ in the shaded region

$= -1$ inside the two circles.

Because of the symmetry, it is equivalent to integration over one circle with a factor 2 . We will evaluate the integral for $\ell = 0, 1, 2$. Since the incident momentum is fixed, let

$k_1 = k_F$, $k_2 = k_F \cos\phi$, where ϕ is the angle between k_1 and k_2,

total momentum $|\bar{k}| = 2\, k_F \cos \phi/2$,

relative momentum $k = k_F \sin \phi/2$.

Total momentum is conserved. The equations of circles are given by

$$\cos^2 \frac{\phi}{2} \pm 2 \cos\theta \cos\frac{\phi}{2} k'' + k''^2 \leq k_F^2 .$$

Let

$$A = P \int_{-1}^{1} P_\ell^2 d\cos\theta \frac{k''^2\, dk''}{k^2 - k''^2}$$

and

$$g(\cos\theta) = \int P_\ell^2 (\cos\theta)\, d\cos\theta .$$

The integration is tedious but straightforward:

$$A = \frac{1}{2\ell + 1} \int_{(1-\cos\phi/2)k_F}^{(1+\cos\phi/2)k_F} \frac{k''^2\, dk''}{k^2 - k''^2}$$

$$+ \int_{(1-\cos\phi/2)k_F}^{(1+\cos\phi/2)k_F} g\left(\frac{k_F^2 \sin^2\frac{\phi}{2} - k''}{2 \sin\frac{\phi}{2}\, k_F\, k''}\right)^2 \frac{k''^2\, dk''}{k^2 - k''^2} \quad \text{(cont.)}$$

$$+ \frac{2}{2\ell + 1} \left(- k'' + \frac{k}{2} \ln \left| \frac{k'' + k}{k'' - k} \right| \right)_0^{(1 - \cos \phi/2)k_F} .$$

To sum up,

$$A = \frac{1}{2\ell + 1} \left[- 2 + \sin \frac{\phi}{2} \ln \left(\frac{1 + \tan \phi/2}{1 - \tan \phi/4} \right) + B_\ell \right. ,$$

where B_ℓ is the second integral in the expression for A, which is to evaluated in Appendix II . The corrected T_ℓ is, from (16),

$$T_\ell = T_0^\ell - \frac{1}{2\pi^2} \left(T_0^\ell \right)^2 (A + B_\ell) .$$

The contribution to m^* from the second term for $\delta(m^*)$ with $m^* = 7$ is about 0.6 . We cannot tell whether it is an acceptable value or not. Since T_0 is qualitatively similar to k in Ref. 11, the correction should be almost the same as calculated in Ref. 2 .

V. CALCULATION OF THE GROUND-STATE ENERGY

Here we calculate the ground-state energy when the T matrix is known. Since it needs more than the two-particle scattering in the Fermi surface, perhaps our effective-mass approximation cannot be expected to be satisfactory. If the density dependence of the forward scattering amplitude in Landau's theory is neglected, our formula will also be applicable there.

The ground-state energy is given in (5):

$$H = \int V \frac{k^2}{2m} G^{<}(k, \omega) d\omega \frac{d^3k}{(2\pi)^4} + \frac{1}{2}\int \Sigma(k, \omega)\, G^{<}(k, \omega) \frac{d\omega\, d^3k}{(2\pi)^4} .$$

If $A(k, \omega) = 2\pi\, \delta(\omega - \omega(k))$ and the effective mass approximation is used, we have

$$H = V\int \frac{k^2}{2m} n(k) \frac{d^3k}{(2\pi)^3} + \frac{1}{2}\int_0^{k_F}\int_0^{k_F} n(k_1)\, n(k_2) \langle k|T|k\rangle \frac{d^3k_1\, d^3k_2}{(2\pi)^6}$$

where

$$n(k) = 1 \qquad \text{if } k \leqslant k_F ,$$

$$n(k) = 0 \qquad \text{if } k > k_F ,$$

and

$$k = \frac{1}{2}\sqrt{k_1^{\,2} + k_2^{\,2} - 2k_1 k_2 \cos\theta} .$$

Since $n(k)$ is a step in the low-temperature limit and we do not know T analytically, we have to change from

$$\int_0^{\pi} d \cos\theta \quad \text{to} \quad 4 \int_{\frac{p_1-p_2}{2}}^{\frac{p_1+p_2}{2}} p \, d \, p$$

and change the order of integration. Furthermore, a factor 2 is added from the summation of spin index in the single-particle Green's function in the second term of H. If we write

$$\int_0^{p_F} dp_1 \int_0^{p_F} dp_2 = 2 \int_0^{p_F} dp_1 \int_0^{p_1} dp_2$$

(17) becomes

$$\frac{8}{\pi^4} \int_0^{p_F} dp \cdot p \left[p \left(\frac{p_F^3 - p^3}{3} \right) - p^2 \left(\frac{p_F^2 - p^2}{2} \right) \right] \left\{ \sum_{\ell \text{ even}} (2\ell+1) + \sum_{\ell \text{ odd}} 3(2\ell+1) \right\} \cdot$$

$$\times \frac{\sin \delta_\ell \cos \delta_\ell}{m^* \, p} .$$

The total number of particles is $N = \frac{1}{3\pi^2} p_F^3$. The single-particle energy is

$$E/N = \frac{3}{5}\left(p_F^2/2m\right) + \frac{24}{\pi}\frac{1}{p_F^3}$$

$$\times \int_0^{p_F} dp \left[p\left(\frac{p_F^3 - p^3}{3}\right) - \frac{p^2\left(p_F^2 - p^2\right)}{2}\right]$$

$$\times \left\{ \sum_{\ell \text{ even}} (2\ell+1) + 3\sum_{\ell \text{ odd}} (2\ell+1) \right\} \frac{\sin\delta_\ell \cos\delta_\ell}{m^*} . \tag{18}$$

If $m^* = 7$ is used and $\delta(m^*)$ is substituted in (18), we have

$$E/N = E_0/N(1 - 1.92) = -2.8^\circ \text{ K} .$$

We are not able to calculate E/N for a range of density to see whether it is the minimum point, since it involves adjustments of p_F, and m^*, two variables. We notice in Refs. 1 and 4 the minimum point is not located at the p_F, which gives the experimental value.

The correction due to a statistical factor makes the value of E/N smaller, but the correction is much less for effective mass, because of the different phase-space factor in (18) .

APPENDIX I

Equations (6) and (8) are derived in Ref. 4; an outline of how to obtain them is given here. Using the Fourier transform of G and T and integrating over time, Eq. (6) becomes ((6') is similar to (6))

$$\left[\left(\frac{\pi\nu}{-i\beta} + k_1^{\,2}/2m - \mu\right) - \lim_{T\to 0} \frac{i}{-i\beta}\, e^{(i\pi\nu/-i\beta)T}\right]$$

$$\times \int \frac{d^3k_2}{(2\pi)^3} \langle k|T\left(\frac{\pi(\nu_1 + \nu_2)}{-i\beta}\right)|k\rangle \cdot G_1\left(k_2, \frac{\pi\nu_2}{-i\beta}\right) \cdot G_1\left(k_1, \frac{\pi\nu_1}{-i\beta}\right) = 1 . \tag{A.1}$$

We neglect T_{12} here . The $\lim_{T\to 0}$ is equivalent to $t_2' \to t_2$ in Eq. (2) . T, T_{12} are the self-energy due to He^3-He^3, He^3-He^4 scattering. Let us consider the part He^3-He^3 only, to simplify the notation:

$$\Sigma_1\left(k_1, \frac{\pi\nu_1}{-i\beta}\right) = -i \int \frac{d^3k_2}{(2\pi)^3} \int \frac{d\omega_2}{2\pi} \frac{A(k_2,\omega_2)}{-i\beta} \sum_{\nu_2}$$

$$\times \frac{e^{\left(i\pi\nu_2/-i\beta\right) T}}{\pi\nu_2/-i\beta - \omega_2} \langle k|T\left(\frac{\pi(\nu_1 + \nu_2)}{-i\beta}\right)|k\rangle \tag{A.2}$$

Here the spectral representation of

$$G(k, \nu) = \int \frac{d\omega_2}{2\pi} \frac{A(k, \omega_2)}{\left(\frac{\pi\nu}{-i\beta} - \omega_2\right)}$$

has been used. To evaluate the summation over V_2, a dispersion relation for T has to be introduced:

$$T(\omega) = i \int \frac{d\omega'}{2\pi} \frac{T(\omega' + i\epsilon) - T(\omega' - i\epsilon)}{\omega - \omega'},$$

$$\text{if } T(\omega) \to 0 \text{ as } \omega \to \infty . \tag{A.3}$$

Using

$$\frac{1}{\frac{\pi\nu_2}{-i\beta} - \omega_2} \cdot \frac{1}{\frac{\pi(\nu_1 + \nu_2)}{-i\beta} - \omega'} = \frac{1}{-\omega_2 + \frac{\pi\nu}{-i\beta} - \omega'} \left[\frac{1}{\frac{\pi\nu_2}{-i\beta} - \omega_2} - \frac{1}{\frac{\pi(\nu_1+\nu_2)}{-i\beta} - \omega'} \right]$$

and

$$\frac{1}{-i\beta}\sum\left(\frac{\pi\nu_1}{-i\beta}-\omega_1\right)^{-1} e^{-i\pi\nu_1\frac{(t_1-t_1')}{-i\beta}} = -i\left(1+e^{-i\omega_1/-i\beta}\right)^{-1} e^{i\omega_1(t_1-t_1')} \quad t_1 > t_1'$$

$$= i\left(1+e^{i\omega_1/-i\beta}\right) e^{i\omega_1(t_1-t_1')} \quad t_1 < t_1'$$

and if ν is taken to be odd in the summation, Eq. (A.2) becomes

$$\Sigma\left(k, \frac{\pi\nu_1}{-i\beta}\right) = +\int \frac{d^3k}{(2\pi)^3} G^<(k_2, \omega_2) \frac{d\omega}{(2\pi)} \langle k|T\left(\frac{\pi\nu_1}{-i\beta}+\omega_2\right)|k\rangle$$

$$+ i\int \frac{d^3k_2}{(2\pi)^3}\int\frac{d\omega_2}{2\pi} G_1\left(k_2, \omega_2 - \frac{\pi\nu_1}{-i\beta}\right)$$

$$\times \frac{\langle k|T(\omega_2+i\epsilon)|k\rangle - \langle k|T(\omega_2-i\epsilon)|k\rangle}{1-e^{i(\omega_2-2\mu)/-i\beta}} . \qquad (A.4)$$

The second term may be regarded as the correction to the Boson behavior of one pair of fermions, and this term will vanish for $\omega_2 \geq 2\mu$ and in the region $\omega_2 \leq 0$, where $\langle T\rangle$ has no cut.

APPENDIX II

B_ℓ is defined as

$$\int_{1-\cos(\phi/2)}^{1+\cos(\phi/2)} g_\ell\left(\frac{\sin^2\frac{\phi}{2} - k''}{2\,k''\cos\frac{\phi}{2}}\right)\frac{k''^2\,dk''}{\sin^2\left(\frac{\phi}{2}\right)-k''^2},$$

where

$$g_\ell(x) = \int p_\ell^{\,2}(x)\,dx\,,$$

$$\ell = 0, \quad B_0 = 1,$$

$$\ell = 1, \quad B_1 = \frac{1}{3}\,\frac{1}{2^3\cos^3\frac{\phi}{2}}\left[2\cos\phi/2 - \left(1-\cos^2\phi/2\right)\ln\left(\frac{1+\cos\phi/2}{1-\cos\phi/2}\right)\right].$$

It is easy to calculate for higher ℓ, but the contribution is too small for $\phi \approx \pi$ where the phase shifts of higher ℓ are large. We notice in the approximation of $T(k) = a$ that the correction is positive in (16), but this is not necessarily true in our case. Furthermore, since the contribution for m^* largely comes from higher ℓ, it makes the correction to m^* relatively small.

ACKNOWLEDGMENT

It is a great pleasure to thank Professor K. M. Watson for his continued interest and suggestions.

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* This work was done under the auspices of the U. S. Atomic Energy Commission.

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Table I.

The phase shifts of the Y-S potential with various mass numbers.

For m = 6

kσ	ℓ						
	0	2	4	6	1	3	5
0.2	-1.06				0.03		
0.4	1.47				0.22		
0.6	1.06	0.03			0.62		
0.8	0.72	0.09			0.90	0.01	
1.0	0.42	0.20			0.95	0.02	
1.2	0.14	0.36	0.01		0.87	0.05	
1.4	-0.11	0.54	0.02		0.74	0.10	
1.6	-0.36	0.65	0.04		0.59	0.17	0.01
1.8	-0.60	0.70	0.06		0.42	0.26	0.02
2.0	-0.84	0.68	0.10	0.01	0.23	0.37	0.03
2.2	-1.07	0.62	0.14	0.02	0.05	0.46	0.05

Table I. continued

For m = 7

kσ	ℓ = 0	2	4	6	1	3	5
0.2	-0.75				0.05		
0.4	-1.35	0.01			0.43		
0.6	1.32	0.03			1.10		
0.8	0.95	0.12			1.30	0.01	
1.0	0.67	0.29			1.24	0.03	
1.2	0.31	0.51	0.01		1.10	0.06	
1.4	0.03	0.73	0.03		0.93	0.13	0.01
1.6	-0.23	0.85	0.05		0.75	0.22	0.02
1.8	-0.48	0.88	0.07	0.01	0.56	0.34	0.03
2.0	-0.73	0.84	0.12	0.01	0.36	0.47	0.04
2.2	-0.97	0.76	0.18	0.02	0.16	0.59	0.05

Table I. continued

For m = 8

kσ	ℓ						
	0	2	4	6	1	3	5
0.2	-0.61				0.11		
0.4	-1.15				1.24		
0.6	1.52	0.04			1.76		
0.8	1.12	0.16			1.69	0.01	
1.0	0.77	0.38			1.51	0.03	
1.2	0.45	0.71	0.01		1.32	0.07	
1.4	0.16	0.97	0.03		1.11	0.15	0.01
1.6	-0.11	1.07	0.05		0.90	0.27	0.02
1.8	-0.38	1.07	0.09	0.01	0.68	0.43	0.03
2.0	-0.63	1.01	0.14	0.02	0.47	0.60	0.04

Table II.

The phase shifts of the 6-12 potential with various mass numbers.

For m = 4

kσ	ℓ = 0	2	4	6	1	3	5
0.2	1.10				0.02		
0.4	0.90				0.11		
0.6	0.66	0.02			0.31		
0.8	0.41	0.06			0.51	0.01	
1.0	0.17	0.13			0.60	0.02	
1.2	-0.05	0.23	0.01		0.59	0.04	
1.4	-0.28	0.34	0.02		0.51	0.07	
1.6	-0.50	0.43	0.03		0.39	0.12	0.01
1.8	-0.70	0.48	0.05		0.25	0.18	0.02
2.0	-0.93	0.48	0.08	0.01	0.10	0.25	0.03
2.2	-1.14	0.45	0.10	0.02	-0.05	0.32	0.04

Table II. continued

For m = 5

kσ	ℓ						
	0	2	4	6	1	3	5
0.2	-1.08				0.02		
0.4	1.46	0.01			0.21		
0.6	1.05	0.03			0.59		
0.8	0.72	0.09			0.87	0.01	
1.0	0.43	0.19			0.93	0.02	
1.2	0.16	0.34	0.01		0.87	0.05	
1.4	-0.02	0.51	0.02		0.75	0.10	
1.6	-0.34	0.62	0.04		0.60	0.17	0.01
1.8	-0.57	0.68	0.06		0.43	0.25	0.02
2.0	-0.80	0.67	0.10	0.01	0.26	0.34	0.03
2.2	-1.02	0.61	0.14	0.02	0.08	0.44	0.05

Table II. continued

For m = 7

kσ	ℓ = 0	2	4	6	1	3	5
0.2	-0.57				0.14		
0.4	-1.09	0.01			-1.50		
0.6	-1.55	0.05			-1.24		
0.8	1.19	0.16			-1.36	0.01	
1.0	0.84	0.40			-1.54	0.03	
1.2	0.53	0.75	0.02		1.39	0.08	
1.4	0.23	1.01	0.03		1.17	0.16	0.01
1.6	0.04	1.12	0.06		0.96	0.27	0.02
1.8	-0.30	1.15	0.09	0.01	0.76	0.43	0.03
2.0	-0.55	1.05	0.14	0.02	0.55	0.61	0.04
2.2	-0.79	0.95	0.21	0.03	0.34	0.75	0.07

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