

## Ground-State Energy and Sound Velocity of a System of Interacting Bosons

V. J. EMERY

*Department of Mathematical Physics, University of Birmingham, England*

J. L. GAMMEL

*Los Alamos Scientific Laboratory, University of California, Los Alamos, New Mexico*

AND

F. R. A. HOPGOOD

*Theoretical Physics Division, Atomic Energy Research Establishment, Harwell, Berkshire, England*

(Received 23 May 1963)

The method of Padé approximants is used to evaluate the ground-state energy  $E_0$  of a system of interacting bosons. The density  $\rho_0$  of particles in the zero-momentum state appears as a free parameter. In particular, the method is applied to a system of hard spheres of radius  $c$  and density  $\rho$ . The result is close to the exact value for low densities and has a singularity at a density which corresponds to close packing when  $\rho_0 = \frac{1}{2}\rho$ . The calculated sound velocity as a function of  $\rho$  coincides with the experimental values for liquid helium II for  $\rho_0 = \frac{1}{2}\rho$  and  $c = 2.16 \text{ \AA}$ .

### I. INTRODUCTION

THE object of this paper is to describe a method of calculating the properties of a system of bosons which may be applicable to liquid helium II.

One approach to this problem is to sum selected terms in perturbation theory<sup>1</sup> and, in this way, it is not too difficult to deal with a weakly interacting system at very high density or a strongly interacting system at very low density—provided the interparticle forces are repulsive. In liquid helium, the forces are strong and partly attractive and the density is neither very high nor very low. If the attractive part of the force were neglected, a combination of the high- and low-density theories could be attempted,<sup>1</sup> but it would be exceedingly difficult to justify the omission of intermediate density terms.

Consequently, although this approach has provided a physical picture of the behavior of liquid helium it needs further modification to produce numerical results in agreement with experiment.<sup>2</sup>

In the method to be described here, *all* terms of a given order of perturbation theory are included and a sequence of Padé approximants<sup>3</sup> is constructed to simulate the behavior of the complete perturbation series. For example, if the ground-state energy per particle  $E_0$  is calculated as a power series in the strength  $V_0$  of the interaction between the particles,

$$E_0 = \sum_{p=0}^{\infty} E_p V_0^p, \quad (1)$$

then the  $(n, m)$  Padé approximant  $P_m^n(V_0)$  is defined as

$$P_m^n(V_0) = \frac{a_0 + a_1 V_0 + a_2 V_0^2 + \cdots + a_n V_0^n}{1 + b_1 V_0 + b_2 V_0^2 + \cdots + b_m V_0^m}, \quad (2)$$

<sup>1</sup> K. A. Brueckner and K. Sawada, Phys. Rev. **106**, 1117, 1128 (1957).

<sup>2</sup> W. E. Parry and D. ter Haar, Ann. Phys. (N. Y.) **19**, 496 (1962).

<sup>3</sup> H. S. Wall, *Continued Fractions* (D. Van Nostrand, Inc., Princeton, New Jersey, 1948).

where the  $a_i$  and  $b_j$  are chosen so that if  $P_m^n(V_0)$  is expanded as a power series in  $V_0$ , the first  $(m+n)$  terms coincide with the first  $(m+n)$  terms in the expansion of  $E_0$ . This prescription defines the  $a_i$  and  $b_j$  uniquely. When expanded,  $P_m^n(V_0)$  contains all powers of  $V_0$  and so gives an approximation to the complete perturbation series which may be useful for very large values of  $V_0$ . In particular,  $P_m^n$  has a finite limit  $a_n/b_n$  as  $V_0 \rightarrow \infty$  so that a hard-core interaction may be dealt with in this way.

Usually, the evaluation of successive terms in a many-body perturbation series is very laborious, but, for an infinite system of bosons, the unperturbed state is extremely simple—every particle has zero momentum—and it is not too difficult to calculate the first few orders in the expansion of the ground-state energy and so to explore the potentialities of the approach before proceeding to discuss other properties and other systems.

In Sec. II the ground-state energy is evaluated to fourth order in perturbation theory and the removal of the divergences characteristic of the many-boson problem is discussed. To this order, it is necessary to introduce an adjustable parameter which is identified with the density  $\rho_0$  of particles in the zero-momentum state. The expressions are evaluated in particular for a finite repulsive core interaction of height  $V_0$  and radius  $c$ . In Sec. III, the Padé approximants  $P_1^1$  and  $P_2^2$  are evaluated in the limit  $V_0 \rightarrow \infty$  to give an estimate of the ground-state energy of a set of hard-sphere bosons as a function of their density  $\rho$ .  $P_2^2(\infty)$  is close to the exact value  $(2\pi\rho c)$  at low densities and also shows a singularity at a density which may be made to correspond to close packing by choice of  $\rho_0$ . The velocity of sound  $u$  calculated from this approximation as a function of  $\rho$  coincides with the experimental values for liquid helium II if  $\rho_0$  is  $\frac{1}{2}\rho$  and  $c$  is  $2.16 \text{ \AA}$ . The rise in  $u$  as  $\rho$  increases is a consequence of the approach to the close packing singularity.

## II. THE PERTURBATION SERIES FOR THE GROUND-STATE ENERGY

The Hamiltonian  $H$  for the system may be separated into unperturbed part  $H_0$  and perturbation  $V$  so that

$$H = H_0 + V \quad (3)$$

and, in second quantization notation,

$$H_0 = \sum_{\mathbf{k}} \frac{1}{2} k^2 a_{\mathbf{k}}^* a_{\mathbf{k}}, \quad (4)$$

$$V = \frac{1}{2\Omega} \sum_{\mathbf{k}, \mathbf{q}, \mathbf{q}'} v(\mathbf{q} - \mathbf{q}') a_{\frac{1}{2}\mathbf{k} + \mathbf{q}}^* a_{\frac{1}{2}\mathbf{k} - \mathbf{q}'}^* a_{\frac{1}{2}\mathbf{k} + \mathbf{q}} a_{\frac{1}{2}\mathbf{k} - \mathbf{q}}. \quad (5)$$

Here, units have been chosen so that  $\hbar = 1$ ,  $m = 1$ , and  $\Omega$  is the normalization volume. The operators  $a_{\mathbf{k}}^*$ ,  $a_{\mathbf{k}}$ , respectively, create and annihilate a particle of momentum  $\mathbf{k}$  and satisfy the commutation relations

$$[a_{\mathbf{k}}, a_{\mathbf{k}'}] = 0 = [a_{\mathbf{k}}^*, a_{\mathbf{k}'}^*], \quad (6)$$

$$[a_{\mathbf{k}}, a_{\mathbf{k}'}^*] = \delta_{\mathbf{k}\mathbf{k}'}. \quad (7)$$

If the potential energy of a pair of particles of separation  $\mathbf{r}$  is given by  $v'(\mathbf{r})$ , then

$$v(\mathbf{k}) = \int d\mathbf{r} v'(\mathbf{r}) e^{-i\mathbf{k}\cdot\mathbf{r}}. \quad (8)$$

The ground state of the unperturbed Hamiltonian is

$$\Delta E_3(1) = \frac{\rho}{\Omega^2} \sum_{\mathbf{q}_1 \neq 0} \sum_{\mathbf{q}_2 \neq 0} v(\mathbf{q}_1) \frac{1}{q_1^2} v(\mathbf{q}_1 - \mathbf{q}_2) \frac{1}{q_2^2} v(\mathbf{q}_2), \quad (13)$$

$$\Delta E_3(2) = \frac{\rho^2}{\Omega} \sum_{\mathbf{q} \neq 0} \frac{v^3(\mathbf{q}) - v^3(0)}{q^4}, \quad (14)$$

$$\Delta E_4(1) = -\frac{1}{2} \frac{\rho}{\Omega^3} \sum_{\mathbf{q}_1 \neq 0} \sum_{\mathbf{q}_2 \neq 0} \sum_{\mathbf{q}_3 \neq 0} \frac{v(\mathbf{q}_1) v(\mathbf{q}_1 - \mathbf{q}_2) v(\mathbf{q}_2 - \mathbf{q}_3) v(\mathbf{q}_3)}{q_1^2 q_2^2 q_3^2}, \quad (15)$$

$$\Delta E_4(2) = -\frac{3\rho^2}{\Omega^2} \sum_{\mathbf{q}_1 \neq 0} \sum_{\mathbf{q}_2 \neq 0} \frac{v(\mathbf{q}_1) v(\mathbf{q}_1 - \mathbf{q}_2)}{q_1^2} \left[ \frac{v^2(\mathbf{q}_2) - v^2(0)}{q_2^4} \right], \quad (16)$$

$$\Delta E_4(3) = -\frac{\rho^2}{\Omega^2} \sum_{\mathbf{q}_1 \neq 0} \sum_{\mathbf{q}_2 \neq 0} \left\{ v^2(\mathbf{q}_1) v(\mathbf{q}_2) [v(\mathbf{q}_2) + v(\mathbf{q}_2 - \mathbf{q}_1)] - \frac{2v^4(0)q_0^2}{q_1^2 q_2^2 + q_0^2} \right\} \frac{1}{q_1^4} \left\{ \frac{2}{q_1^2 + q_2^2 + (\mathbf{q}_1 - \mathbf{q}_2)^2} - \frac{1}{q_2^2} \right\}, \quad (17)$$

$$\Delta E_4(4) = -\frac{2\rho^2}{\Omega^2} \sum_{\mathbf{q}_1 \neq 0} \sum_{\mathbf{q}_2 \neq 0} \left\{ \frac{v(\mathbf{q}_1) v(\mathbf{q}_2) [v(\mathbf{q}_1 - \mathbf{q}_2) + v(\mathbf{q}_1)] [v(\mathbf{q}_2) + v(\mathbf{q}_1 - \mathbf{q}_2)]}{q_1^2 q_2^2 [q_1^2 + q_2^2 + (\mathbf{q}_1 - \mathbf{q}_2)^2]} - \frac{4v^4(0)q_0^2}{q_1^2 + q_2^2 + q_0^2} \frac{1}{q_1^2 q_2^2 [q_1^2 + q_2^2 + (\mathbf{q}_1 - \mathbf{q}_2)^2]} \right\}, \quad (18)$$

$$\Delta E_4(5) = -\frac{5}{2} \frac{\rho^3}{\Omega} \sum_{\mathbf{q} \neq 0} \frac{v^4(\mathbf{q}) - v^4(0)}{q^6}, \quad (19)$$

obtained by putting every particle in the plane-wave state of zero momentum and it is this fact which makes the problem reasonably tractable.

Many-body perturbation theory and its application to a Bose gas has been reviewed in some detail by Brueckner<sup>4</sup> and the details will not be repeated here.

The characteristic feature of the perturbation theory of a Bose gas is that beyond second order, there occur terms which diverge in the limit of infinite volume as a consequence of the dominant role played by the zero momentum state. One of the objects of the method introduced by Brueckner and Sawada<sup>1</sup> is to remove this divergence by a partial summation of terms from all orders of perturbation theory.

If the divergent parts are separated out in each order then the first four terms of the perturbation series are

$$\Delta E_1 = \frac{1}{2} \rho v(0), \quad (9)$$

$$\Delta E_2 = -\frac{1}{2} \frac{\rho}{\Omega} \sum_{\mathbf{q} \neq 0} \frac{v^2(\mathbf{q})}{q^2}, \quad (10)$$

$$\Delta E_3 = \Delta E_3(1) + \Delta E_3(2) + \Delta E_3^D(0), \quad (11)$$

$$\Delta E_4 = \Delta E_4(1) + \Delta E_4(2) + \Delta E_4(3) + \Delta E_4(4) + \Delta E_4(5) + \Delta E_4^D(0), \quad (12)$$

where  $\rho$  is the number density and

<sup>4</sup> *The Many Body Problem*, edited by C. Dewitt (Dunod Cie, Paris, 1959).

$$\Delta E_3^D(\epsilon) = \frac{\rho^2}{\Omega} \sum_{q_1 \neq 0} \frac{v^3(0)}{(q^2 + \epsilon^2)^2}, \quad (20)$$

$$\begin{aligned} \Delta E_4^D(\epsilon) = & -\frac{3\rho^2}{\Omega^2} \sum_{q_1 \neq 0} \sum_{q_2 \neq 0} \frac{v(\mathbf{q}_1)v(\mathbf{q}_1 - \mathbf{q}_2)v^2(0)}{q_1^2(q_2^2 + \epsilon^2)^2} - \frac{2\rho^2}{\Omega^2} \sum_{q_2 \neq 0} \sum_{q_1 \neq 0} \frac{v^4(0)q_0^2}{q_1^2 + q_2^2 + q_0^2} \frac{1}{(q_1^2 + \epsilon^2)^2} \left\{ \frac{2}{q_1^2 + q_2^2 + (q_1 - q_2)^2 + \epsilon^2} - \frac{1}{q_2^2 + \epsilon^2} \right\} \\ & - \frac{8\rho^2}{\Omega^2} \sum_{q_2 \neq 0} \sum_{q_1 \neq 0} \frac{v^4(0)q_0^2}{q_1^2 + q_2^2 + q_0^2} \frac{1}{(q_1^2 + \epsilon^2)(q_2^2 + \epsilon^2)[q_1^2 + q_2^2 + (q_1 - q_2)^2 + \epsilon^2]} - \frac{5\rho^3}{2\Omega} \sum_{q \neq 0} \frac{v^4(0)}{(q^2 + \epsilon^2)^6}. \quad (21) \end{aligned}$$

$\Delta E_3$  and  $\Delta E_4$  have been rearranged in this way so that  $\Delta E_3^D(0)$  and  $\Delta E_4^D(0)$  are the only terms which diverge in the limit of infinite volume. The quantity  $q_0^2 \times (\mathbf{q}_1^2 + \mathbf{q}_2^2 + \mathbf{q}_0^2)^{-1}$  has been included to ensure convergence of the sums for high momenta. Since it replaces  $v(\mathbf{q})$  in this role,  $q_0$  should be of the order of the reciprocal of the range of  $v'(r)$ .

One method of dealing with the divergences would be to replace  $\Delta E_3^D(0)$  and  $\Delta E_4^D(0)$  by  $\Delta E_3^D(\epsilon)$  and  $\Delta E_4^D(\epsilon)$ , respectively, in Eqs. (11) and (12), then to form the Padé approximants and finally to let  $\epsilon$  tend to zero. However, in order to obtain a significant result from this procedure, it is necessary to work to a much higher order in perturbation theory.

Consequently, it is better to adopt the alternative approach of summing selected terms from the divergent parts of higher orders of perturbation theory so as to leave a finite value of  $\epsilon$  in the energy denominators. This procedure has been carried out by Brueckner and Sawada<sup>1</sup> who show that for  $\Delta E_3^D(\epsilon)$  and the  $\rho^3$  term of  $\Delta E_4^D(\epsilon)$ , a first approximation for  $\epsilon$  is given by

$$\epsilon^2 = 8\pi\rho_0 a, \quad (22)$$

where  $\rho_0$  is the density of particles in the zero momentum state<sup>2</sup> and  $a$  is the scattering length of the interaction. The value of  $\epsilon$  which should be used in the  $\rho^2$  terms of  $\Delta E_4^D(\epsilon)$  is not given by Eq. (22) but the difference should not be too large and it will be neglected. In this approach, there is no prescription for calculating  $\rho_0$  and it will be treated as a free parameter. If  $a < 0$ , Eq. (22) cannot be used and  $\epsilon$  must be treated as a free parameter.

The scattering length  $a$  may be expressed as a power series in the coupling constant so if Eq. (22) is used to define  $\epsilon$  and  $\Delta E_3^D(\epsilon)$  is expanded in powers of the coupling constant, there will be a fourth-order contribution which should be subtracted from  $\Delta E_4^D(\epsilon)$ . To lowest order,  $\rho_0$  may be replaced by  $\rho$  and the result is that the factor  $(-\frac{5}{2})$  in the  $\rho^3$  term of  $\Delta E_4^D(\epsilon)$  has to be replaced by  $(\frac{5}{2})$ .

The simplest case of some physical interest is a system of hard spheres, whose behavior is well understood at very high and very low densities. The potential,  $v'(r)$ , is given by

$$\begin{aligned} v'(r) &= V_0 \quad \text{for } r \leq c, \\ &= 0 \quad \text{for } r > c, \end{aligned} \quad (23)$$

and after the formation of the Padé approximants,  $V_0$  will be allowed to become infinite. For finite  $V_0$ , the scattering length is given by

$$a = c - \frac{\tanh V_0^{1/2} c}{V_0^{1/2}}, \quad (24)$$

which becomes equal to  $c$  when  $V_0 \rightarrow \infty$ .  $q_0$  is to be set equal to  $c^{-1}$ .

In the limit of infinite volume, the sums in Eqs. (9) to (21) become integrals of which only  $\Delta E_4(3)$ ,  $\Delta E_4(4)$  and those which contain  $q_0$  in  $\Delta E_4^D(\epsilon)$  have to be evaluated numerically. In particular,  $\Delta E_1$ ,  $\Delta E_2$ ,  $\Delta E_3(1)$ , and  $\Delta E_4(1)$  are the first four terms in the expansion of  $2\pi\rho a$  and can be determined by expanding the right-hand side of Eq. (24) in powers of  $V_0$ .

The results are

$$E_1 = \Delta E_1 V_0^{-1} = \frac{2\pi}{3} \rho c^3, \quad (25)$$

$$E_2 = \Delta E_2 V_0^{-2} = -\frac{4\pi}{15} \rho c^5, \quad (26)$$

$$E_3 = \Delta E_3 V_0^{-3} = \frac{34\pi}{315} \rho c^7 - \frac{6231\pi^2}{16800} \rho^2 c^{10} + \frac{8\pi^2}{27} \frac{\rho^2 c^9}{\epsilon}, \quad (27)$$

$$\begin{aligned} E_4 = \Delta E_4 V_0^{-4} = & -\frac{124\pi}{2835} \rho c^9 + 3.064 \rho^2 c^{12} - 11.34 \rho^3 c^{15} \\ & - \frac{16\pi^2}{45} \frac{\rho^2 c^{11}}{\epsilon} + \frac{8\pi^3}{27} \frac{\rho^3 c^{14}}{\epsilon} - \frac{20\pi^3}{81} \frac{\rho^3 c^{12}}{\epsilon^3} - I(\epsilon). \end{aligned} \quad (28)$$

$I(\epsilon)$  has to be found numerically for each value of  $\epsilon$ . For small values of  $\epsilon$ ,

$$I(\epsilon) \approx \left[ \left( \frac{\sqrt{3}}{4} \pi - \frac{1}{3} \pi^2 \right) \ln(\epsilon^2 c^2) - 5.566 \right] \frac{64}{81} \rho^2 c^{12}. \quad (29)$$

### III. PADÉ APPROXIMATION

The first diagonal Padé approximant  $P_1^1(V_0)$  of the perturbation series for the energy is given by

$$P_1^1(V_0) = \frac{2\pi}{3} \rho c^3 \frac{V_0}{1 + \frac{2}{3} c^2 V_0} \quad (30)$$

$$\rightarrow \frac{5}{6} (2\pi\rho c) \quad (31)$$

as  $V_0 \rightarrow \infty$ . This result may be compared with the low-density limit of  $2\pi\rho c$  obtained by Lee, Huang, and Yang.<sup>5</sup> It is clearly inadequate at all but the lowest densities.

The second Padé approximant  $P_2^2(V_0)$  has the form

$$P_2^2(V_0) = \frac{a_0 + a_1 V_0 + a_2 V_0^2}{1 + b_1 V_0 + b_2 V_0^2}. \quad (32)$$

The method of calculating the  $a_i$  and  $b_j$  from  $E_1$ ,  $E_2$ ,  $E_3$ , and  $E_4$  is described in Sec. I and it is found that

$$\lim_{V_0 \rightarrow \infty} P_2^2(V_0) = \frac{a_2}{b_2} = \frac{2E_1 E_2 E_3 - E_2^3 - E_1^2 E_4}{E_2 E_4 - E_3^2} \quad (33)$$

which may be evaluated with the aid of Eqs. (25) to (28) and Eq. (22). The numerator and denominator of the result may each be reduced to the sum of a polynomial of fourth degree in  $(\rho c^3)^{1/2}$  and a term depending upon  $\ln(\rho c^3)$ . The coefficients depend upon  $\rho_0$ .

In Fig. 1,  $P_2^2(\infty)$  is shown as a function of  $(\rho c^3)^{-1/3}$  for several values of  $\rho_0$ . It has a quite different behavior from  $P_1^1(\infty)$ . The discussion of Fig. 1 will be separated into three parts.

### A. Low Densities

Here  $\rho_0 \rightarrow \rho$  and

$$P_2^2(\infty) = 2\pi\rho c \frac{14}{15} \left\{ \frac{1 + 1110.3(\rho c^3)^{1/2} + \dots}{1 + 1208.5(\rho c^3)^{1/2} + \dots} \right\}. \quad (34)$$

Clearly, there is no point in expanding this expression in powers of  $(\rho c^3)^{1/2}$  and the second term of the expansion would not coincide with the exact expression.<sup>5</sup> However, the numerical value is close to the low-density limit of  $2\pi\rho c$ . The very large coefficients of  $(\rho c^3)^{1/2}$  occur because both numerator and denominator had to be multiplied by large factors to make their leading terms unity. This feature is a consequence of the fact that the coefficients  $a_2$  and  $b_2$  in the  $P_2^2$  approximant of the expansion of  $a$  in Eq. (24) are very small.

### B. High Densities

$E_0$  should have a double pole<sup>6</sup> at the close packing density

$$\rho c^3 = \sqrt{2}. \quad (35)$$

As can be seen from Fig. 1,  $P_2^2$  has a singularity but it is a simple pole. Of course, at close packing, a given particle interacts strongly with twelve other particles so that an approximation based upon fourth-order perturbation theory and thus including no more than four-body collisions with any accuracy would not be ex-

<sup>5</sup> T. D. Lee, K. Huang, and C. N. Yang, Phys. Rev. **106**, 1135 (1957).

<sup>6</sup> F. London, *Superfluids* (John Wiley & Sons, Inc., New York, 1954), Vol. II.

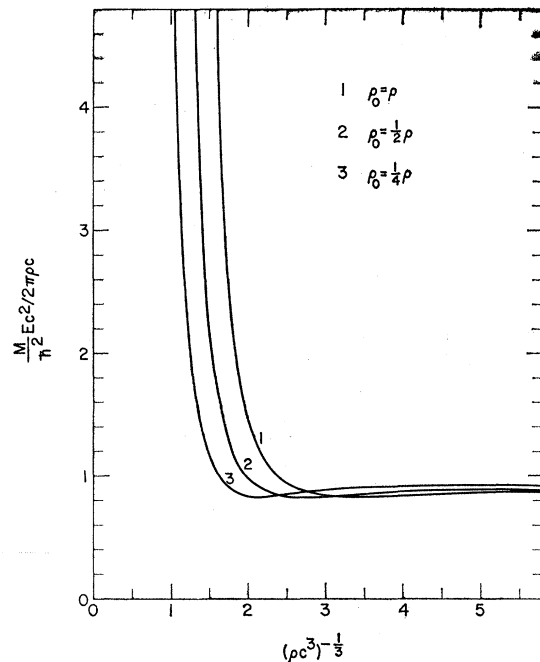


FIG. 1. The second diagonal Padé approximation  $P_2^2(\infty)$  to the energy divided by the exact low-density limit  $2\pi\rho$ .  $\rho_0$  is the density of particles in the zero-momentum state and, for liquid helium II,  $(\rho c^3)^{-1/3}$  is about 1.6.

pected to be valid. Nevertheless, for  $\rho_0 = \frac{1}{4}\rho$ , the singularity in  $P_2^2$  occurs at the density given by Eq. (35).

Higher Padé approximants are unlikely to introduce a double pole but may have a second pole at a density somewhat higher than that for close packing.

### C. Liquid-Helium Densities

On the basis of the Keesom-Taconis<sup>7</sup> model of liquid helium, one may estimate crudely that a given helium atom interacts simultaneously with about six others, although the structure is considerably less rigid than that of a close packed crystal. Consequently,  $P_3^3$  could be a good approximation at liquid-helium densities and  $P_2^2$  may not be too inaccurate.

One quantity which may be calculated for a system of hard spheres and compared with experiments on liquid helium is the sound velocity  $u$  given by

$$u^2 = \frac{d}{d\rho} \left( \rho^2 \frac{dE_0}{d\rho} \right). \quad (36)$$

$c$  is to be interpreted as an effective hard-core radius which should be rather less than the radius, 2.56 Å, of the repulsive part of the interaction between helium atoms. The calculation may be regarded as an attempt to estimate  $\rho_0$  and  $c$  for liquid helium by choosing them to fit the experimental values of  $u$  as a function of  $\rho$ .

If the pressure of liquid helium is varied from the

<sup>7</sup> W. H. Keesom and K. W. Taconis, Physica **4**, 28, 256 (1937); **5**, 270 (1938).

vapor pressure to 25 atm, the density increases by about 15% and, at 1.25°K, the sound velocity increases from 237 m/sec to 365 m/sec. From Eq. (36) it follows that this increase in the value of  $u$  may be attributed to the rise in  $E_0$  as close packing density is approached. Since  $\rho$  varies by such a small amount, it is most reasonable to choose  $\rho_0$  and  $c$  to fit the mean experimental values of  $u$  and  $du/d\rho$ . For  $c=2.16$  Å and  $\rho_0=\frac{1}{2}\rho$ , the calculated and measured values of  $u$  agree to within a few percent. These values of  $\rho_0$  and  $c$  are close to those estimated by Parry and ter Haar<sup>2</sup> on the basis of the theory of Brueckner and Sawada.<sup>1</sup>

#### IV. CONCLUSIONS

The Padé approximant  $P_2^2$  gives a good qualitative representation of  $E_0$  for all densities and by choice of very plausible values of  $\rho_0$  can be made to give quite

accurate numerical results. To estimate the accuracy of the approximation within the framework of the method itself, it would be necessary to go to sixth-order perturbation theory in order to compare  $P_3^3$  with  $P_2^2$ .

However, the results from fourth-order perturbation theory are sufficiently encouraging to suggest that it would be worthwhile to calculate the energy spectrum in the same way and to introduce the true interaction between helium atoms.

#### ACKNOWLEDGMENTS

Part of this work was carried out while two of the authors (V.J.E. and J.L.G.) were visitors in the Theoretical Physics Division at A.E.R.E. Harwell, England and they wish to acknowledge the hospitality of Dr. W. Marshall.

## Fluxoid Quantization, Pair Symmetry, and the Gap Energy in the Current-Carrying Bardeen-Cooper-Schrieffer State\*†

MURRAY PESHKIN

*Argonne National Laboratory, Argonne, Illinois*

(Received 20 May 1963)

The method of Byers and Yang is extended for application to the current-carrying BCS state by including the magnetic interaction between electrons in the zero-order Hamiltonian. In the case of a thin superconducting ring, the problem is reduced to the zero-current problem by separating out the collective motion. In the general case, this process is not carried out completely, but the symmetry of the BCS state provides enough information to obtain the desired results. When the fluxoid is equal to an integral multiple of  $(\pi\hbar c/e)$ , the single-particle states occur in pairs which go into each other under reflection about the average electron velocity at each point. A qualitative argument is given to show why this symmetry is necessary for the BCS reduced interaction to have its full effectiveness. The crux of the matter is that in the absence of such symmetry, the Fermi surface is irregular and a substantial fraction of the important states near that surface are unable to participate in a coherent BCS wave function. The Meissner effect is not necessary for the quantization of magnetic flux.

### 1. INTRODUCTION

THE atomic theory of Bardeen, Cooper, and Schrieffer<sup>1,2</sup> (BCS) provides a generally satisfactory description of the zero-current state in a superconductor. However, in dealing with the supercurrent state, in which the magnetic interaction between the electrons is of the first importance, it has customarily been necessary to resort to phenomenological methods. The atomic understanding of the zero-resistance, or

persistent-current phenomenon, remains, in this respect, incomplete or at best obscure. Thus, the fact that the trapped flux threading a superconducting ring is quantized in multiples of  $(\pi\hbar c/e)$  had to be discovered experimentally,<sup>3,4</sup> although it is in reality a simple consequence of the BCS theory.

The connection between flux quantization and the BCS theory was first explained by Byers and Yang.<sup>5</sup> These authors consider a ring superconductor whose thickness is much greater than its penetration depth, so that the Meissner effect is complete. They exclude the surface regions, where the currents actually flow, from

\* Work performed under the auspices of the U. S. Atomic Energy Commission.

† This work was reported briefly at the St. Louis Meeting of the American Physical Society [M. Peshkin, *Bull. Am. Phys. Soc.* **8**, 191 (1963)].

<sup>1</sup> J. Bardeen, L. M. Cooper, and J. R. Schrieffer, *Phys. Rev.* **108**, 1175 (1957).

<sup>2</sup> N. N. Bogoliubov, V. V. Tolmachev, and D. V. Shirkov, *A New Method in the Theory of Superconductivity* (Consultants Bureau, Inc., New York, 1959).

<sup>3</sup> B. S. Deaver, Jr., and W. M. Fairbank, *Phys. Rev. Letters* **7**, 43 (1961).

<sup>4</sup> R. Doll and M. Nabauer, *Phys. Rev. Letters* **7**, 51 (1961).

<sup>5</sup> N. Byers and C. N. Yang, *Phys. Rev. Letters* **7**, 46 (1961). Similar results were obtained by J. M. Blatt, *Progr. Theoret. Phys. (Kyoto)* **26**, 721 (1961).