

Exchange Energy in bcc $^3\text{He}^\dagger$

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(Received 16 June 1969)

Values of the exchange energy J for bcc ^3He have been obtained from the exchange contribution to the pressure in measurements extending to 13 mK. The relation between the exchange energy and the pressure is developed. A brief outline of the experimental arrangement including a description of a simple procedure for obtaining ^3He of fairly high purity is given. The data analysis and uncertainty in J are discussed. Values of $|J|$ are given and compared with other determinations. It is found for the solid near melting ($V=24.1\text{ cm}^3/\text{mole}$), that $|J|/k=0.72\text{ mK}$, with a strong volume dependence $\partial \ln|J|/\partial \ln V \approx 18$. Assuming antiferromagnetic ordering, the Néel temperature for the solid near melting would be $T_N=2.0\text{ mK}$. The specific heat, entropy, and thermal expansion of the solid are considered. A brief comment concerning ^4He impurities is made.

I. INTRODUCTION

Since the early speculation on nuclear-spin ordering in solid ^3He by Pomeranchuk,¹ there has been much interest in this subject. Pomeranchuk considered only the dipole-dipole interaction of a rigid lattice and concluded that ordering would not take place until about 10^{-6} K . It was pointed out by Bernardes and Primakoff² that ordering should occur at a much higher temperature because of the exchange interaction resulting from the large zero-point motion in the solid. Recently, theoretical calculations^{3,4} of the exchange energy J have been made which give $J/k \sim -0.1\text{ mK}$, indicating antiferromagnetic ordering.

Attempts at experimental determination of the ordering temperature fall into two categories. The first is through observation of some equilibrium thermodynamic property such as magnetic susceptibility or specific heat. Earliest efforts using this approach were the susceptibility measurements of Fairbank and co-workers.^{5,6} These did not give reliable results, primarily because of the unexpectedly large effects of ^4He impurities and because the temperatures were not low enough. The susceptibility study was continued by Meyer *et al.*⁷ and, although this work did not give accurate values for the ordering temperature, the indication was that the ordering should be antiferromagnetic. Quite recently, further susceptibility studies^{8,9} have been made but these have only set upper limits on the ordering temperature. This has also been the case with the specific-heat work.¹⁰

Another approach to the determination of J , which has been more successful, has been through its relation to the longitudinal and trans-

verse nuclear relaxation times. This method has the advantage that measurements may be made at a much higher temperature $\sim 1\text{ K}$. A number of such studies have been made,¹¹⁻¹⁵ the most recent and systematic being by Richards, Hatton, and Giffard¹⁴ and by Richardson, Hunt, and Meyer¹⁵ (RHM). Although the agreement on the value of J in these two most recent studies^{14,15} has been to within about a factor of 2, values differing by almost a factor of 10 have been reported.¹²

From the above discussion, the desirability of a direct equilibrium determination of J is apparent. In addition to the susceptibility and specific heat, the expansion coefficient or pressure offers another possibility for this. Such a determination of J through its effect on the pressure of the sample was made possible by recent refinements in strain gauge techniques for measuring small pressure changes.¹⁶ Application of this technique was made by us recently¹⁷ to obtain J for molar volumes near melting. With further improvement in sensitivity it has now been possible to study smaller molar volumes. This paper presents extension of the work to most of the bcc phase.

In Sec. II, we develop the relation between the exchange energy and the pressure. (No discussion of the theory of the exchange interaction is given; the reader is referred to the papers by Nosanow and Varma³ and by Guyer.⁴) A brief discussion is given of the experimental arrangement, data analysis and error, followed by the results and conclusion.

II. EXCHANGE CONTRIBUTION TO THE PRESSURE

The definition of the exchange energy per pair

J is in terms of the difference in energy between the singlet and triplet states^{3,4}

$$2J = E_s - E_t. \quad (1)$$

The exchange Hamiltonian is written in the usual Heisenberg form, which has been shown to be valid for solid ³He,¹⁸

$$H_{\text{ex}} = -2 \sum_{i < j} J \vec{I}_i \cdot \vec{I}_j, \quad (2)$$

where \vec{I} is the nuclear-spin operator and the subscript ex stands for exchange. Ferromagnetic or antiferromagnetic ordering corresponds to $J > 0$ or $J < 0$, respectively. [It should be noted that the above is the conventional way of defining J . Much of the NMR work^{12, 14, 15} omits the factor of 2 in Eq. (2). This difference in definition must be taken into account in comparing results.]

Various thermodynamic quantities of interest are evaluated through the partition function

$$Z_{\text{ex}} = \text{Tr} \exp(-H_{\text{ex}}/kT). \quad (3)$$

The series expansion of $\ln Z_{\text{ex}}$, valid for $T > T_N$, as given by Baker *et al.*¹⁹ is

$$\ln Z_{\text{ex}} = N \ln 2 + N \sum_{n > 0} \frac{e_n}{2^n n!} \left(\frac{J}{kT} \right)^n, \quad (4)$$

where N is the number of particles and the e_n are coefficients. For a bcc lattice, the first few of these are¹⁹ $e_1 = 0$, $e_2 = 12$, $e_3 = -24$, and $e_4 = 168$.

The exchange contribution to the pressure is given by

$$p_{\text{ex}} = kT \left(\frac{\partial \ln Z_{\text{ex}}}{\partial V} \right)_T, \quad (5)$$

where V is the volume. Substituting the partition function of Eq. (4) and using the indicated coefficients, we have

$$p_{\text{ex}} = N \left[3 \left(\frac{J}{kT} \right) \frac{\partial J}{\partial V} - \frac{3}{2} \left(\frac{J}{kT} \right)^2 \frac{\partial J}{\partial V} + \dots \right]. \quad (6)$$

As it turns out, the maximum value of $|J/k|$ is ≈ 1 mK. Therefore, since the lowest temperature reached in this work is 13 mK, we need only the high-temperature limit of this in which only the first term is kept. For the purpose of analyzing the data, it is convenient to write the first term in (6) in the form

$$p_{\text{ex}} = \frac{3R}{V} \left(\frac{J}{k} \right)^2 \frac{\partial \ln |J|}{\partial \ln V} \frac{1}{T}, \quad (7)$$

where R is the gas constant, and V now refers to molar volume. We point out that in Eq. (7) only the magnitude of J is determined. If the measurements were extended to $T \approx 7$ mK, the sign of J would be revealed from the second term in (6). Also the sign of J may be obtained from measurements of p_{ex} in a magnetic field. Although it does not affect any of our results, in this paper we assume $J < 0$. Further work is needed to establish this more firmly.

In the above discussion, only the exchange contribution to the pressure has been considered. There will be an additional contribution due to phonons, which, for a Debye solid, would be

$$p_{\text{ph}} = -\frac{3\pi^4 R}{5V} \frac{\partial \ln \theta_D}{\partial \ln V} \frac{T^4}{\theta_D^3}, \quad (8)$$

where θ_D is the Debye temperature. The exchange and phonon contributions to p become equal at $T \sim 0.2$ K. Since the ratio $p_{\text{ph}}/p_{\text{ex}}$ varies as T^5 , the phonon term becomes negligible very rapidly at lower temperatures.

III. EXPERIMENTAL

The experiment consisted of measurements of pressure versus temperature for various constant-volume samples, with J to be extracted using Eq. (7) above. A brief description of the apparatus and techniques was given previously,¹⁷ and a full exposition will appear elsewhere.²⁰ Only a few details will be given here. Pressures of the samples were measured by means of a capacitive strain gauge.^{16, 17} The only significant changes from the gauge used previously¹⁷ was the use of Be-Cu instead of stainless steel, with design improvements which permitted detection of pressure changes of $\Delta p \approx 2 \times 10^{-6}$ atm.

Because of the previously mentioned effects of ⁴He impurities, it was desired that the ³He sample be of high purity. Samples with a ⁴He concentration $x = 2 \times 10^{-5}$ were obtained by the simple expediency of distillation in the evaporator of a cyclic (continuous) ³He refrigerator. The initial concentration of ⁴He was $x \approx 5 \times 10^{-4}$. In order to purge the external refrigerator plumbing of impure gas, the refrigerator was allowed to run overnight during which time ⁴He impurity accumulated in the evaporator. Then, about half the ³He in the refrigerator was evaporated at $T \sim 0.3$ K and was used for the sample. With greater care, samples with $x \sim 10^{-6}$ could probably be obtained in this way.

Samples were formed at constant volume, using the blocked capillary method. In order to remove pressure inhomogeneities produced by this method, the samples were then annealed at about 0.01 K below the melting temperature. Since the annealing

process affected the sample pressure, the process could be observed and was considered to be completed when the pressure reached a steady value (at fixed T). For all molar volumes studied, the annealing time was 30 min or less. After the annealing process further changes in temperature took place slowly.

Temperatures as low as 13.3 mK were reached by demagnetization of 175 g of chromium potassium alum from 0.3 K and 13 kG. A zinc heat switch was used to connect the sample chamber to the salt. This permitted the sample temperature to be raised above that of the salt and to be regulated electronically using the salt as a heat sink. With this arrangement, data could be taken while warming or cooling, or the sample temperature could be held constant for several hours. The ballistically measured susceptibility of 10 g of powdered cerium magnesium nitrate (CMN) served as a thermometer. Contact to the CMN was through 2000 #44 copper wires which provided an area of contact of 160 cm². The thermal time constant between the CMN and the ^3He sample was never longer than 5 min. Since the warming rate due to heat leaks was only about 0.2 mK/h at the lowest temperature, this time constant never presented any problem in achieving good thermal equilibrium between the CMN and the ^3He .

IV. DATA ANALYSIS AND ERROR

The raw data were taken as capacitance C of the strain gauge versus galvanometer deflections δ for the CMN thermometer. For the pressure changes of roughly 10^{-2} atm or less due to the exchange, a linear relation between pressure and C was valid. Also we have $\delta \propto 1/T$. Thus, a plot of C versus δ is equivalent to p_{ex} versus $1/T$ except for scale changes. In order to determine the coefficient

$$\frac{3R}{V} \left(\frac{J}{k} \right)^2 \frac{\partial \ln |J|}{\partial \ln V}$$

in Eq. (7), all that is required is the slope of the straight line through the raw C -versus- δ data with the appropriate changes in scale. Typical data are shown in Fig. 1 where C versus δ was plotted with the scales changed to correspond to p versus $1/T$. It is seen that the linear relation expected from Eq. (7) is observed for $T \lesssim 0.1$ K.

Data such as those shown in Fig. 1 were taken for about 10 different molar volumes between 21.0 and 24.2 cm³/mole. For each volume, the slope

$$\frac{3R}{V} \left(\frac{J}{k} \right)^2 \frac{\partial \ln |J|}{\partial \ln V}$$

of p_{ex} versus $1/T$ was evaluated. Since the slope

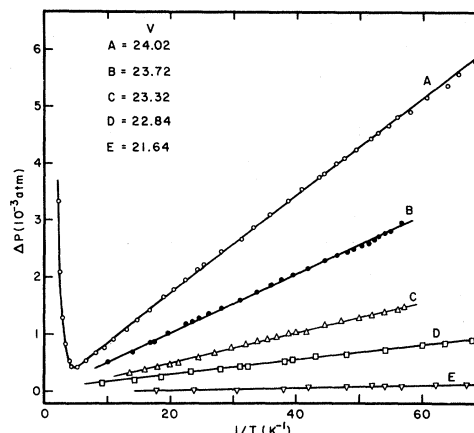


FIG. 1. Pressure difference versus T^{-1} for various molar volumes. For $V = 24.02$ cm³/mole the high-temperature phonon contribution is shown. For the other volumes, the T^{-1} exchange contribution only is shown. From the slopes in the T^{-1} region, values of the exchange energy are obtained.

involves J and its derivative, the slope for a single molar volume is not sufficient to evaluate $|J|$. But, with data for several volumes, a self-consistent procedure allows $|J|$ to be determined. An initial arbitrary value of $\partial \ln |J| / \partial \ln V$ is chosen and $|J(V)|$ evaluated for each volume. With this $|J(V)|$, a new value of $\partial \ln |J| / \partial \ln V$ is found and used to compute a new $|J(V)|$. This is repeated until a self-consistent value is obtained for $|J(V)|$. As it turns out, $\partial \ln |J| / \partial \ln V$ is very nearly constant and the process requires only one or two cycles. The final values of $|J(V)|$ are independent of the initial value of $\partial \ln |J| / \partial \ln V$ used.

The above procedure for determining $|J(V)|$ is subject to two sources of error. The first is experimental error in the slopes of p_{ex} -versus $1/T$. The second is in the self-consistent analysis. The correctness of Eq. (7), obtained from the series expansion of the partition function using the Heisenberg Hamiltonian to represent the spin system, is assumed.

The experimental error in converting galvanometer deflections δ to $1/T$ is estimated to be about 1%. The error in converting ΔC to Δp is negligible since absolute pressures are not required, only pressure differences. For the largest molar volumes, where Δp_{ex} is ~ 1000 times the smallest detectable pressure change, the error in determination of the slope of ΔC versus δ is only about 1 or 2%. At smaller molar volumes the error in this slope becomes greater, being about 15% at 22 cm³/mole and 30% at 21 cm³/mole. But, since the slope is proportional to J^2 , the corresponding error in $|J|$ is about $\frac{1}{2}$ this.

In the self-consistent procedure for solving for $|J|$, discussed above, the error occurs in deter-

mining the best value of $\partial \ln |J| / \partial \ln V$. The line through our data in Fig. 2 has a slope $\partial \ln |J| / \partial \ln V \approx 17.5$ at $V=24$ and 19.2 at $V=22$. The data are fitted almost as well by a straight line with a slope of 18 . Again, because the difference occurs in J^2 , this makes a relatively small difference in $|J|$. The $|J(V)|$ computed for the constant slope are about 1% smaller at $V=24$ and about 3% larger at $V=22$. Then, from all sources, we estimate the uncertainty in $|J|$ to be $<3\%$ for $V=24$ and about 8 and 15% for $V=22$ and 21 cm^3/mole , respectively.

V. RESULTS AND DISCUSSION

The values of $|J(V)|$ obtained as indicated above are shown in Fig. 2. Other results are shown for comparison, including theoretical calculations,^{3,4} results obtained from NMR work,^{14,15} and our previous results.¹⁷ Correction of a computational error in the work of RHM has been taken into account.²¹ The slight difference between our present values and those reported earlier¹⁷ is primarily due to the difference in $\partial \ln |J| / \partial \ln V$ which is now better defined. The agreement between the NMR values of RHM and those of this work is quite good. In view of the vast differences in two methods, this close agreement is particularly gratifying.

Once $|J|$ has been determined, various thermodynamic properties of ^3He which are related to $|J|$ may be evaluated. Of particular interest is the antiferromagnetic transition temperature T_N . Various numerical factors connecting T_N and $|J|/k$ have been given. The relation found by Baker *et al.*¹⁹ is

$$T_N = 2.75 |J|/k. \quad (9)$$

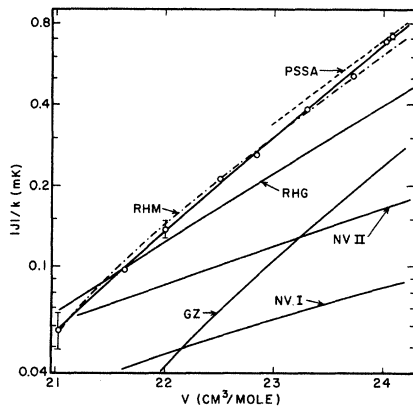


FIG. 2. Exchange energy versus molar volume. Circles and the unlabeled solid line, this work; PSSA, Ref. 17; RHM, Ref. 15; RHG, Ref. 14; NVI and II, theory, Ref. 3; GZ, theory, Ref. 4.

The largest realizable Néel temperature will be for the solid at the melting pressure at $T \approx 0$, which should be²⁰ for $V \approx 24.1$ cm^3/mole . We find $|J|/k = 0.72$ mK for this molar volume, resulting in a maximum value of $T_N = 2.0$ mK. (The solid exists at V as large as about 24.8 cm^3/mole with $|J|/k \approx 1.2$ mK and $T_N \approx 3.3$ mK. However, since this solid melts at $T \lesssim 0.32$ K, the higher T_N cannot be observed.) In recent compressional cooling of ^3He , a temperature $T^* = 2.15$ mK has been reached,²² which is very near our $T_N = 2.0$ mK.

In the high-temperature limit $T \gg T_N$, the magnetic susceptibility is expected to obey the Curie-Weiss law, $\chi = C/(T + \Theta)$, with $\Theta = 4|J|/k$.²³ For $V = 24.1$ cm^3/mole , this gives a maximum observable Θ of 2.9 mK. At the present time, susceptibility measurements⁷⁻⁹ have not been made to low enough temperatures with sufficient precision to confirm this behavior.

Other thermodynamic quantities such as the entropy and specific heat may be obtained using the high-temperature series expansions.¹⁹ For convenience, we give these

$$\frac{S}{R} = \sum_{n \geq 0} \frac{(1-n)e_n}{2^n n!} \left(\frac{J}{kT}\right)^n, \quad (10)$$

$$\text{and } \frac{C}{R} = \sum_{n \geq 0} \frac{n(n-1)e_n}{2^n n!} \left(\frac{J}{kT}\right)^n, \quad (11)$$

where $e_0 = \ln 2$ and other coefficients through e_4 were given, previously. With the $|J(V)|$ found in this work, values of S and C may be computed, using Eqs. (10) and (11) where it is to be assumed that $J < 0$. The entropy of the solid at melting is of particular significance since it is one of the determining factors in the slope of the melting curve. This situation has been discussed by Scribner *et al.*²⁰

The thermal expansion coefficient α is related to the pressure by the relation $\alpha = k_T(\partial p / \partial T)_V$, where k_T is the compressibility. Just as does the pressure, this has two contributions, one obtained from Eq. (7) due to exchange, the other obtained from Eq. (8) due to phonons. Since $\partial \ln |J| / \partial \ln V > 0$ the contribution to α due to exchange is negative, while that due to phonons is positive.¹⁶ Therefore, for a given molar volume, the expansion coefficient will be zero at some temperature where the two contributions are equal in magnitude with negative values below and positive above (see Fig. 1, $V = 24.02$). This has been pointed out and considered extensively by Goldstein.²⁴

For large molar volumes, the position of the zero of α is fairly well defined experimentally by the minimum in $p = p_{\text{ex}} + p_{\text{ph}}$ and can be located with ease (see Fig. 1, $V = 24.02$). For $V \lesssim 22$ cm^3/mole , $\alpha \approx 0$ over a wide temperature interval and the zero is not well defined experimentally. Mathemat-

ically, the position of $\alpha = 0$ can be found by setting

$$\frac{\partial}{\partial T} \dot{p}_{\text{ex}} = -\frac{\partial}{\partial T} \dot{p}_{\text{ph}}$$

from Eqs. (7) and (8). This was done to locate the zero of α for $V < 22 \text{ cm}^3/\text{mole}$. In Fig. 3, the regions of positive and negative expansion coefficients in the solid are shown on the p - T phase diagram. For completeness, the melting curve and the sign of α for the liquid²⁵ are shown. In the solid, the intersection of the line $\alpha = 0$ with the melting curve occurs at $T = 0.21 \text{ K}$. From analysis of the exchange energy¹⁷ and phonon specific heat,²⁶ Goldstein²⁴ finds this intersection at 0.23 K and an intersection with the bcc-hcp phase boundary at 0.073 K .

From the above discussion, it is seen that the influence of spin ordering on the thermal expansion or pressure extends to relatively high $T \approx 200 \times |J|/k \approx 0.2 \text{ K}$. This favorable situation for observing the effect of spin ordering on α or p is a result of the large value of $\partial \ln |J| / \partial \ln V \approx 18$ compared to $-\partial \ln \theta_D / \partial \ln V \approx 2$. In contrast, the exchange specific heat should equal that due to phonons at $T \approx 0.14 \text{ K}$. Furthermore, in the susceptibility we should expect only a 5% departure from Curie's law at $T \approx 0.04 \text{ K}$. Thus, unless very precise measurements are made, the susceptibility requires much lower temperatures than the pressure measurements for studying spin ordering.

Finally, we comment briefly on the situation regarding ^4He impurities. As we stated earlier, in this study the ^4He concentration was $x = 2 \times 10^{-5}$. These samples would undergo phase separation²⁷⁻²⁹ at $T_{\text{ps}} \approx 0.07 \text{ K}$. For the concentration involved here, the maximum value of the excess pressure²⁸ due to phase separation is $< 10^{-4} \text{ atm}$ and not observable on the scale of Fig. 1. Assuming that the phase separation removes the ^4He impurity from the bulk of the ^3He sample, the sample purity would increase with decreasing temperatures. (Because of the long time constants for

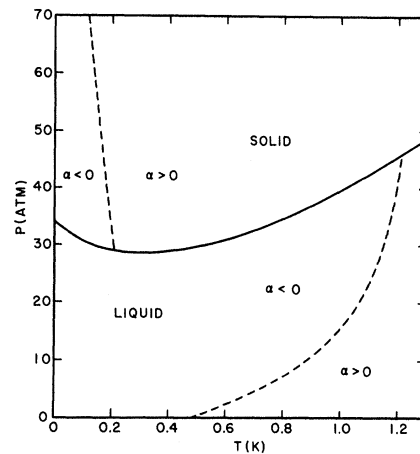


FIG. 3. Phase diagram showing the regions of positive and negative expansion coefficients in the solid and liquid.

phase separation, this would not occur for $V \lesssim 22 \text{ cm}^3/\text{mole}$.) At $T = 0.047 \text{ K}$, the ^4He impurity in the ^3He -rich phase is reduced to only 10^{-7} . Therefore, if the presence of ^4He impurities of $x \lesssim 2 \times 10^{-5}$ has any marked effect on J which is observable in \dot{p}_{ex} , we should find the slope of \dot{p}_{ex} versus $1/T$ to be different above and below $T_{\text{ps}} = 0.07 \text{ K}$. From Fig. 1, it is seen that \dot{p}_{ex} versus $1/T$ is a straight line over the entire temperature range $\lesssim 0.15 \text{ K}$ with no change in slope below T_{ps} . Thus, we believe that the values of $|J|$ obtained are for pure ^3He .

ACKNOWLEDGMENTS

We wish to thank R. A. Scribner for assistance in the initial phase of this work. We are grateful to L. H. Nosanow and C. M. Varma and to R. A. Guyer and L. I. Zane for furnishing us the results of their theoretical calculations prior to publication. We acknowledge useful discussions with Louis Goldstein.

[†]Research supported by the National Science Foundation.

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Series Expansion in the Variational Approach to Many-Boson Problems*

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(Received 27 January 1969)

The ground state of a many-boson system is studied within the range of the Bijl-Dingle-Jastrow-type description when the radial distribution function $g(r)$ differs little from its asymptotic value. The treatment of the problem is based on the development of power series in $\alpha = 1 - g(0)$ for all physical quantities which depend on the particle density. The n -particle distribution functions $p^{(n)}$ are evaluated to order α^4 as functionals in the $g(r)$ function for $n=3$ and 4 using the cluster-expansion procedure outlined by Abe. These results are used in connection with the improvement of the ground-state description when the wave function is not the optimum choice. Using $p^{(3)}$ function obtained, the Bogoliubov-Born-Green-Kirkwood-Yvon equation is solved, also to order α^4 , for the two-particle correlation function $\mathfrak{U}(r)$, and the first two leading corrections to the hypernetted-chain (HNC) approximation are obtained. The variational calculation along with the series expansion for $\mathfrak{U}(r)$ yields formulas for the ground-state properties, including some corrections to known results. For a charged boson gas, numerical values of $\mathfrak{U}(r)$, $p^{(3)}$, $p^{(4)}$, and the ground-state energy are computed using the Gaussian approximation for $g(r)$, and the results show that the errors associated with the HNC approximation are small. A brief discussion is presented on the method of determining the general expansion coefficients of the correlation functions of $p^{(n)}$ in terms of $g(r)$.

I. INTRODUCTION

In recent years, the theoretical study of a many-particle boson problem has been approached with

a great variety of approximation methods. In particular, the variational procedure based on the Bijl-Dingle-Jastrow (BDJ) type of correlated trial wave function of the form