

Crossover from Fermi Liquid to Classical Behavior of Normal ^3He in the Model of Almost Localized Fermions

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A phenomenological extension of the model of almost localized fermions to finite temperatures is presented. It is used to calculate thermodynamic properties of the normal state of ^3He . No new adjustable parameters are introduced and the effective interaction strength is the same as used by Vollhardt. A good qualitative description of the crossover from Fermi liquid to classical behavior in the specific heat, spin susceptibility, and temperature-dependent pressure (or equivalently thermal expansion) is obtained. In particular, key results, such as the change in specific heat when the spin entropy saturates and the change from thermal expansion to thermal contraction at low temperatures are reproduced.

1. INTRODUCTION

The model of almost localized fermions proposed for normal ^3He by Anderson and Brinkman¹ and extensively studied by Vollhardt² gives a good description of the thermodynamic functions in the Fermi liquid regime. The physical basis for this model is the assumption that ^3He is a liquid close to localization or solidification. A similar assumption has been discussed by Castaing and Nozières,³ who proposed a nearly solid structure for the strongly spin-polarized state of ^3He . Andreev and Kosevich⁴ applied a similar description to the higher temperature classical regime. A natural question that arises is whether one can extend the almost localized model to describe the crossover from Fermi liquid behavior at low temperatures

to classical behavior at higher temperatures. Only one adjustable parameter—the strength of the effective short-range repulsion—was needed to describe the Fermi liquid behavior at $T = 0$ K. Our goal is to extend the model to higher temperatures without introducing any further adjustable parameters. The extension to higher temperatures is essentially phenomenological, as indeed is the almost localized model itself, and follows from the work of Rice *et al.*⁵ They applied the model to the specific heat and entropy of heavy fermion systems. Normal ^3He is, however, a more severe test of the model, since there are more measurements, namely specific heat (or equivalently entropy), spin susceptibility, and pressure at constant volume (or equivalently thermal expansion). A unified description of these three thermodynamic properties is the goal of this work.

The thermodynamic properties of ^3He are particularly interesting since they vary on the scale of a reduced Fermi temperature T_F^* , which is considerably smaller than the bare Fermi temperature T_F . A comprehensive set of high-precision data on the specific heat and the specific volume was reported recently by Greywall.⁶ These data confirm that the properties are not simply given by a rescaled free fermion behavior. The explanation of these properties has attracted the attention of a number of workers. The unusual behavior in the specific heat has been ascribed to an enhancement of the effective mass in a limited region of \mathbf{k} space near the Fermi wave vector due to coherent particle-hole excitations.⁷ Others have stressed the importance of spin-fluctuation excitations. Brown *et al.*⁸ have argued that the data could only be explained by a strong temperature variation of the effective mass due to the decoupling of higher energy quasiparticles from low-lying spin-fluctuation excitations. The approach, however, that is closest to ours is the recent work of Mishra and Ramakrishnan,⁹ who have extended the paramagnon, or almost ferromagnetic, model to higher temperatures. They discussed first the spin susceptibility and recently the specific heat by separating spin and density fluctuations. The former dominate for temperatures $T \lesssim T_F^*$. There are two essential parameters in their approach, namely a susceptibility enhancement as $T \rightarrow 0$ and a cutoff in \mathbf{k} space for the spin fluctuations. In the almost localized model the effective interaction plays the role of the first parameter, but there is no equivalent of the second parameter. Instead, there is a natural cutoff due to the finite bound on the entropy of the local spin fluctuations ($\sim k_B \ln 2$ per ^3He atom). Thus it is an essential condition for the applicability of the almost localized model that the anomalous behavior in the specific heat is associated with the bound of $R \ln 2$ on the spin fluctuation entropy. As we shall see below, ^3He fulfills this entropy condition, and this fact, together with the explanation of the constancy of the ratio of spin susceptibility to specific heat as $T \rightarrow 0$ (Wilson ratio ~ 4), are definite successes of the almost localized model.

The bound of $R \ln 2$ on the entropy was used by Goldstein¹⁰ some time ago (i.e. before Landau's Fermi liquid theory). He proposed a theory of liquid ^3He based on a separation into spin and nonspin contributions to thermodynamic properties. Introducing the notion of an internal field in the liquid, he assumed that only those spins N_σ that had "freed" themselves from this field contributed to the spin susceptibility $\chi = \mu_0^2 N_\sigma / T$ ($k_B = 1$) and at the same time yielded a spin entropy $S = N_\sigma \ln 2$ because of the spin- $\frac{1}{2}$ character of the ^3He atoms. In this way he linked the spin susceptibility to the entropy, which in turn allowed him to calculate the specific heat. Because of the bounded entropy, the spin contribution to the specific heat was necessarily found to have a pronounced peak. Goldstein assumed that this peak would indirectly show up in the total heat capacity c_v . Indeed, the sharp kink in the c_v versus T curves, for example, at ~ 0.2 K at high pressures, appears to be due to this very structure.

In the picture of almost localized fermions that we propose, the entropy is bounded by $R \ln 2$ only for temperatures $T_F^* \leq T \ll U$ (U is the effective short-range interaction), because in this temperature range essentially only singly occupied lattice sites exist. Note, however, that the behavior for $T > T_F^*$ is not simply that of free fermions. The singlet or density excitations have a characteristic energy U and while the coherent Fermi liquid properties are lost on a scale of T_F^* , free fermion behavior is not recovered so long as $T < U$. There are thus two quite different characteristic temperature scales in liquid ^3He .

We point out that the aim of our work is to describe the crossover from Fermi liquid to classical behavior at $T \sim T_F^*$ and that the description of the initial corrections to the Fermi liquid behavior may not be so accurate. These corrections have been much studied in the paramagnon model and Béal-Monod *et al.*¹¹ have shown that the T^2 term in the susceptibility accurately obeys a paramagnon scaling law. This is also the case in our results; however, the numerical coefficient is considerably larger than in the experiment.

Concerning the specific heat in our model, an analytic expansion in a power series in T does not give a $T^3 \log T$ term. In the paramagnon model such a nonanalytic term was found by Doniach and Engelsberg¹² as well as by Berk and Schrieffer.¹³ Later it was shown by Pethick and Carneiro¹⁴ that the $T^3 \log T$ term can be computed within Landau Fermi liquid theory. While in paramagnon theory the $T^3 \log T$ contribution should only be observable at very low temperatures, the recent measurements by Greywall⁶ seem to indicate* that such a term persists up to temperatures of the

*We should point out that the temperature range of the $T^3 \log T$ fit to Greywall's data is limited, i.e., less than a decade, and there are substantial deviations at very low temperatures due to experimental uncertainties.

order of 200 mK at low pressures. A theoretical explanation for this has recently been put forward by Coffey and Pethick.¹⁵ On the other hand, our interest is to describe the behavior of c_v on a larger temperature scale and to go through the crossover to classical behavior.

In addition to the spin susceptibility and specific heat we will also examine the temperature dependence of the pressure at constant volume $P(T)|_V$. Usually one considers the volume at fixed pressure, i.e., the thermal expansion. Helium-3 is unusual in that at low temperatures there is an initial contraction at $T \lesssim 1$ K and an expansion only for $T \gtrsim 1$ K. Greywall⁶ has recently presented a comprehensive series of experimental data on this point. He presents his data as $P(T)|_V$ so that the anomalous expansion shows up as a minimum in $P(T)|_V$ at finite T . In contrast, for free fermions this quantity is monotonically increasing. The almost localized model reproduces the minimum and even gives good quantitative agreement as the pressure $P \rightarrow P_c$, the solidification pressure.

The outline of the paper is as follows. In Section 2 we present an extension to finite temperature of the almost localized fermion model. In Section 3 we discuss the appropriate form of the model for ^3He . The key point here is the role of higher energy excitations, which we include in the simplest possible way, namely as free fermions. Then in Sections 4–6 we present the results of our model calculations for the specific heat and entropy, spin susceptibility, and $P(T)|_V$ in the temperature range $T \lesssim 2.5$ K and at volumes corresponding to $P = 0, 15, 30$ bar at $T = 0$. Finally Section 7 has some concluding remarks.

2. GENERALIZATION OF THE ALMOST LOCALIZED FERMION MODEL

We start this section by reviewing the Gutzwiller theory for almost localized Fermi systems. A more complete account can be found in the recent review by Vollhardt.² For the Hubbard Hamiltonian with a repulsive on-site interaction U Gutzwiller¹⁶ proposed the following variational ground-state wave function:

$$\psi_G(\{n(\mathbf{k}, \sigma)\}, g) = \prod_i [1 - (1 - g)n_{i\uparrow}n_{i\downarrow}] \Phi_0(\{n(\mathbf{k}, \sigma)\}) \quad (1)$$

Here Φ_0 is the ground state of the uncorrelated system (i.e., a Slater determinant) and $n_{i\sigma}$ is the number operator for site i and spin σ . The occupation numbers in Φ_0 have values $n(\mathbf{k}, \sigma) = 1$ for $k < k_F$ and 0 otherwise ($T = 0$). The physical idea behind the ansatz (1) is that, due to the strong repulsive interaction, the number of doubly occupied sites is reduced with respect to Φ_0 .

After minimization with respect to the variational parameter g , Gutzwiller obtained an approximate expression for the ground-state energy per site as

$$E_G = \sum_{\mathbf{k}\sigma} q_{\sigma}(d, n_{\sigma}) \varepsilon_{\mathbf{k}\sigma} n(\mathbf{k}, \sigma) + Ud \quad (2)$$

Here d and n_{σ} are the concentrations of doubly occupied sites and of singly occupied sites with spin σ , respectively. The sum over \mathbf{k} states is normalized to 1. The function q is given in terms of d and n_{σ} as

$$q_{\sigma}(d, n_{\sigma}) = \{[(1 - n_{\sigma} - n_{-\sigma} + d)(n_{\sigma} - d)]^{1/2} + [d(n_{-\sigma} - d)]^{1/2}\}^2 \times [n_{\sigma}(1 - n_{\sigma})]^{-1} \quad (3)$$

The factor q renormalizes the kinetic energy in (2) and can be interpreted as the enhancement of the effective mass m^* over the bare mass m ($q^{-1} = m^*/m$). Also, the discontinuity of the momentum distribution at the Fermi energy is reduced from 1 to q . Extracting the Landau parameters from the energy expression (2) leads to a good agreement with experimental results, provided the density of states is chosen properly. We will come back to this point in the next section.

The case of a half-filled band ($n_{\sigma} = n_{-\sigma} = 1/2$) has been studied by Brinkman and Rice.^{17,18} They found that with increasing U , the fraction of doubly occupied sites d decreases from its value of $d = 1/4$ in the uncorrelated state to $d = 0$ at a critical interaction strength $U_c (= 8|\bar{\varepsilon}_0|$, with $\bar{\varepsilon}_0 = \sum_{\mathbf{k} < k_F, \sigma} \varepsilon_{\mathbf{k}\sigma}$), i.e., the fermions localize in the Mott sense. This half-filled band case in the almost localized limit ($U < U_c$, $U_c - U \ll U_c$) has been used by Anderson and Brinkman¹ and Vollhardt² to describe the static properties of normal ³He at zero temperature. We will see that, as temperature fluctuations of the occupation number become important, we have to allow for a filling factor slightly less than 1, i.e., $n_{\sigma} + n_{-\sigma} = 1 - \delta$, with $\delta \ll 1$. In this case the system never becomes completely localized, but for large U , $d \rightarrow 0$ and $q \approx 2\delta$.

Most recently the assumption of a half-filled band ($\delta = 0$) for $T = 0$ at all pressures was examined by Vollhardt *et al.*¹⁹ by using a model with variable density. They showed that, on energy grounds, an increase of the external pressure (i.e., approaching the transition) leads to $\delta \rightarrow 0$, justifying the assumption made earlier in ref. 2.

An extension to higher temperature has been presented recently by Rice *et al.*⁵ Excited state wave functions can be obtained from the Gutzwiller form (1) by varying the occupation numbers $\{n(\mathbf{k}, \sigma)\}$. The internal energy can then be calculated in the same way as in (2). To obtain the free energy we need an expression for the entropy. For this purpose we must recognize that the set of excited states determined by varying $\{n(\mathbf{k}, \sigma)\}$ are not mutually

orthogonal, because of the projection operator. On the other hand, we can easily calculate the total number of independent states with a fixed value of d , using a real space representation. In the case $\delta = 0$ this number varies continuously from 4 per site in the uncorrelated state ($d = \frac{1}{4}$) to 2 per site in the almost localized limit ($d \rightarrow 0$). In addition we know from Landau Fermi-liquid theory that the low-energy excitations are quasiparticles whose entropy is determined by the free fermion entropy formula. This leads to the following ansatz for the entropy:

$$S = - \sum_{\mathbf{k}\sigma} w(\mathbf{k}, d, n_\sigma) \{ n(\mathbf{k}, \sigma) \ln n(\mathbf{k}, \sigma) + [1 - n(\mathbf{k}, \sigma)] \ln [1 - n(\mathbf{k}, \sigma)] \} \quad (4)$$

Here $w(\mathbf{k}, d, n_\sigma)$ is a weighting function in \mathbf{k} space to account for the above-mentioned overcompleteness.

The occupation number is obtained by minimizing the free energy F ,

$$F = \sum_{\mathbf{k}, \sigma} q_\sigma \varepsilon_{\mathbf{k}\sigma} n(\mathbf{k}, \sigma) + Ud - TS \quad (5)$$

with respect to $\{n(\mathbf{k}, \sigma)\}$ and we get

$$n(\mathbf{k}, \sigma) = \{ \exp [q_\sigma (\varepsilon_{\mathbf{k}\sigma} - \mu_\sigma) / w(\mathbf{k}, d, n_\sigma) T] + 1 \}^{-1} \quad (6)$$

Note that the quantity $w(\mathbf{k}, d, n_\sigma) q_\sigma^{-1}$ in (6) plays the role of a \mathbf{k} -dependent effective mass. On physical grounds we can derive three constraints on the w -function:

1. To reproduce Landau theory we impose the constraint on w that

$$\lim_{k \rightarrow k_F} w(\mathbf{k}, d, n_\sigma) = 1 \quad (7)$$

2. For sufficiently high temperatures, i.e., for $T > T_F^*$ ($= qT_F$) but $T \ll U$ and $q \ll 1$ (almost localized limit) the occupation number $n(\mathbf{k}, \sigma)$ approaches the limiting value $(1 - \delta)/2$ and the entropy per site becomes

$$S = \bar{w} [\ln 4 - (1 - \delta) \ln(1 - \delta) - (1 + \delta) \ln(1 + \delta)] \quad (8)$$

with

$$\bar{w}(d, n_\sigma) = \sum_{\mathbf{k}} w(\mathbf{k}, d, n_\sigma) \quad (9)$$

On the other hand, it is simple to calculate the total number of degrees of freedom with fixed values of d and n_σ in a site representation (see, for example, Vollhardt²). Comparing these two results, we get the following entropy sum rule for the weighting function $w(\mathbf{k}, d, n_\sigma)$:

$$\bar{w} = - \frac{(1 - \delta - 2d) \ln[\frac{1}{2}(1 - \delta) - d] + d \ln d + (d + \delta) \ln(d + \delta)}{\ln 4 - (1 - \delta) \ln(1 - \delta) - (1 + \delta) \ln(1 + \delta)} \quad (10)$$

In the limit $d, \delta \rightarrow 0$, \bar{w} takes the value $1/2$.

Therefore we see that on the temperature scale T_F^* a total molar entropy $\sim R \ln 2$ is obtained. This is what one expects for an almost localized fermion regime. For higher temperatures as $T \gg T_F^*$ one finds

$$d(T) \approx \frac{1}{2}[1 + \exp(U/2T)]^{-1} \quad (11)$$

Thus it is only on the higher temperature scale of $U/2$ that $d \rightarrow \frac{1}{4}$, as expected for free fermions. In this limit $S(T)$ approaches $R \ln 4$, i.e., the maximum entropy of fermions in a model with a limited bandwidth. Therefore in the interval $T_F^* < T < U/2$ the system has lost Fermi liquid coherence but is not yet a free fermion system, since it is still well below the second intrinsic temperature scale.

3. Later, when discussing the spin susceptibility, we will also derive a sum rule for the inverse of the weighting function:

$$\bar{w}_{-1}(d, n_\sigma) = \sum_{\mathbf{k}} (1/w(\mathbf{k}, d, n_\sigma)) = 2(1 - 2d - \delta) \quad (12)$$

Our procedure then is to parametrize the w -function as simply as possible, consistent with the three conditions (5), (10), and (12), and with a fixed choice of the w -function to calculate the thermodynamic properties. We expect that the results will be insensitive to the detailed form of w -functions.

A somewhat similar approach to a finite temperature extension of a variational ansatz á la Gutzwiller was proposed by Spátek *et al.*²⁰ However, instead of choosing a function $w_{\mathbf{k}}$ in the expression for S [Eq. (8)], these authors used only a single parameter describing the fraction of itinerant particles. We cannot see that the above-mentioned entropy requirements (i.e., *three* conditions on $w_{\mathbf{k}}$) can be fulfilled by this one parameter.

3. THE MODEL FOR HELIUM-3

The main problem in applying the almost localized model to ${}^3\text{He}$ is the unlimited density of states of such a liquid, in contrast to the limited bandwidth of the Hubbard model. Our approach will be to treat the states near the Fermi energy as strongly correlated, while the higher energy states are considered to be free and uncorrelated. The choice of which states are free and which states are correlated is fixed by the requirement that as $T = 0$ the model reduces to the half-filled band model of Anderson and Brinkman¹ and Vollhardt.² Therefore we define a cutoff energy E_c such that the number of states with $E < E_c$ is exactly twice the number of states with $E < E_F$. The states with $E < E_c$ are treated in the almost localized fermion model, while those with $E > E_c$ are taken to be free.

For finite temperatures the filling factor is reduced from half-filled according to

$$\delta(T) = \int_{E_c}^{\infty} dE f(E) N_f(E) \quad (13)$$

Here $f(E)$ is the Fermi function and $N_f(E)$ is the density of states (DOS) for free fermions.

There are two problems with the above DOS. First, the sharp cutoff, which was chosen for simplicity, is clearly artificial and a more gradual transition from strongly correlated to free would be physically more reasonable. Second, an uncertainty lies in the p factor of this square-root DOS. This factor, introduced by Vollhardt,² is defined as $p = 2|\bar{\epsilon}_0|N(E_F)$. For the square-root DOS, $p = 1.2$, while for the half-ellipse DOS used by Vollhardt, $p = 1.08$. The Wilson ratio, R_W , is very sensitive to the precise value of p . Within the almost localized model R_W can be calculated to be $(1 - 3p/4)^{-1}$ at the localization transition. The experimentally measured value of R_W corresponds to a value $p = 1$, while for $p = 1.2$, $R_W = 10$. Although it is not quite clear which lattice structure would represent the short-range order in ³He best, we will also choose a half-ellipse DOS for the strongly correlated states around the Fermi energy. It should be noted² that any bounded, symmetric DOS that somehow resembles a half-ellipse (e.g., that for a simple cubic lattice) always yields a value for p very close to $p = 1.08$, i.e., is insensitive to the detailed structure of the lattice. In dimensionless units with $E_F = 1$ the DOS of the correlated states $N_c(E)$ is fully determined by the two conditions $\int dE N_c(E) = 1$ and $N_c(E_F) = N_f(E_F)$. Explicitly,

$$N_c(E) = \frac{3}{2} \{1 - [(E - 1)/\Delta]^2\}^{1/2}, \quad 1 - \Delta \leq E \leq 1 + \Delta \quad (14)$$

with $\Delta = 8/3\pi$.

The free states for $E \geq E_c$ are described by the usual square-root DOS

$$N_f(E) = \frac{3}{2} E^{1/2}, \quad E \geq E_c \quad (15)$$

The total DOS is shown in Fig. 1. In the following we change the variables $(\mathbf{k}, d, n_\sigma) \rightarrow (E, d, \delta, m)$, where $\delta = 1 - n_\sigma - n_{-\sigma}$ and $m = n_\sigma - n_{-\sigma}$.

For the w -function we make the three-parameter ansatz

$$w(E, d, \delta) = A \exp[-(E - 1)^2/R^2] + B \quad (16)$$

A careful examination of the sum rules (5), (10), and (12) shows that w is approximately independent of m . The quantities A , B , and R are functions of d and δ via the sum rules. From (5) it follows that $B = 1 - A$. For a discussion of the energy and magnetization dependence of w in (16) see Appendix B.

We will make calculations for three different molar volumes: 36.84, 28.86, and 26.14 cm³. The values of d at $T = 0$ were determined by Vollhardt²

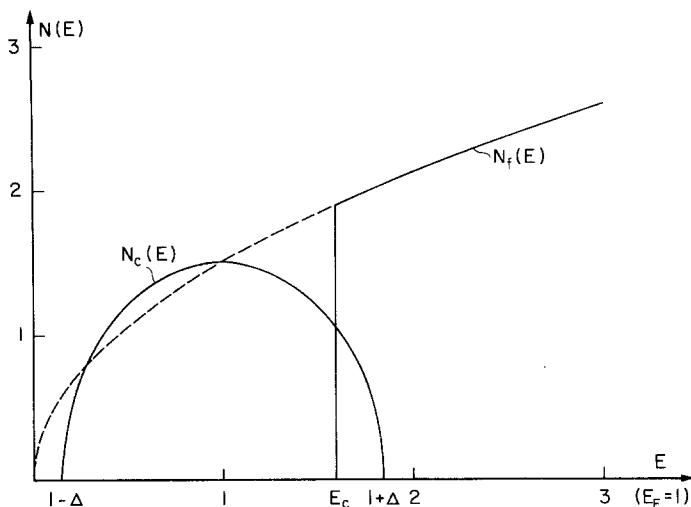


Fig. 1. The density of states used for the numerical calculations. $N_c(E)$ is the assumed form of the DOS for the correlated states as described in the text. $N_f(E)$ describes the free and uncorrelated states.

by fitting the linear term in the specific heat at each pressure. For simplicity we put $d(T) = d(0) \equiv d_0$ in the temperature range of interest, namely $T \approx T_F^*$ but $T \ll U$. Also, A and R are kept constant as a function of temperature. We checked the validity of these approximations, and, as discussed below, they are not serious. Note the remarks made in Appendix A and B on the approximation $d = \text{const}$.

The values of the quantities of interest are given in Table I.

4. THE SPECIFIC HEAT AND THE ENTROPY

The specific heat at a constant volume is defined by the equation $c_v = T(\partial S/\partial T)_{V,N}$. Using the entropy expression (4), it is straightforward

TABLE I^a

V, cm^3	d	T_F, K	A	R	U	$V \partial d/\partial V$
26.14	0.024	6.23	0.78	0.44	2.60	0.068
28.86	0.032	5.84	0.87	0.52	2.52	0.075
36.84	0.050	4.96	1.27	0.77	2.31	0.084

^a A , R , and U are given in units with $T_F=1$. The value of T_F is calculated with the formula $T_F = (\hbar^2/2m)(3\pi^2 N/V)^{2/3} = 54.91 V^{-2/3}$ K. The stationary condition for the free energy at $T=0$ leads to $U = 8|\bar{\epsilon}_0|(1-4d)$.

to obtain [$n_{\mathbf{k}} \equiv n(\mathbf{k}, \sigma)$]

$$\begin{aligned} c_v^c &= \left(\frac{q}{T}\right)^2 \sum_{\mathbf{k}\sigma} n_{\mathbf{k}}(1-n_{\mathbf{k}})(\varepsilon_{\mathbf{k}}-\mu) \left(\varepsilon_{\mathbf{k}}-\mu + T\frac{\partial\mu}{\partial T}\right) / w_{\mathbf{k}} \\ &= \left(\frac{q}{T}\right)^2 \int dE N_c(E) n(E-\mu) [1-n(E-\mu)] (E-\mu) \\ &\quad \times \left(E-\mu + T\frac{\partial\mu}{\partial T}\right) / w(E) \end{aligned} \quad (17)$$

The superscript c indicates that this is the contribution of the correlated states alone.

Particle conservation requires

$$\int dE N_c(E) n(E-\mu) + \int dE N_f(E) f(E-\mu) = 1 \quad (18)$$

From this equation we can self-consistently calculate the chemical potential μ and δ for each temperature. Taking the derivative of (18) with respect to T then gives a closed expression for $\partial\mu/\partial T$:

$$T\frac{\partial\mu}{\partial T} = -\frac{qI_1^c + I_1^f}{qI_2^c + I_2^f} \quad (19)$$

where

$$I_1^c = \int dE N_c(E) n(E-\mu) [1-n(E-\mu)] (E-\mu) / [Tw(E)] \quad (20)$$

$$I_2^c = \int dE N_c(E) n(E-\mu) [1-n(E-\mu)] / [Tw(E)] \quad (21)$$

I_1^f and I_2^f are the corresponding expressions for the free part, i.e., $q = w = 1$, $\int_{1-\Delta}^{1+\Delta} dE \rightarrow \int_{E_c}^{\infty} dE$, $N_c(E) \rightarrow N_f(E)$, $n(E-\mu) \rightarrow f(E-\mu)$.

For higher temperatures (17) is no longer sufficient, since then the free states are partially populated and contribute a considerable amount to the total specific heat:

$$c_v = c_v^c + c_v^f \quad (22)$$

The free part of the specific heat c_v^f is given by a formula analogous to (17) again with $q = w - 1$, $\int_{1-\Delta}^{1+\Delta} dE \rightarrow \int_{E_c}^{\infty} dE$, $N_c(E) \rightarrow N_f(E)$, and $n(E-\mu) \rightarrow f(E-\mu)$.

In Fig. 2 we show a plot of the calculated and measured specific heat c_v for the three different molar volumes (36.84, 28.86, 26.14) cm^3 that correspond to the zero-temperature pressures $P(0) = 0, 15, 30$ bar. Note that there is *no* additional fitting parameter involved. The only free parameter is d_0 , or equivalently U/U_c , which was used to give the experimental value of c_v/T as $T \rightarrow 0$.

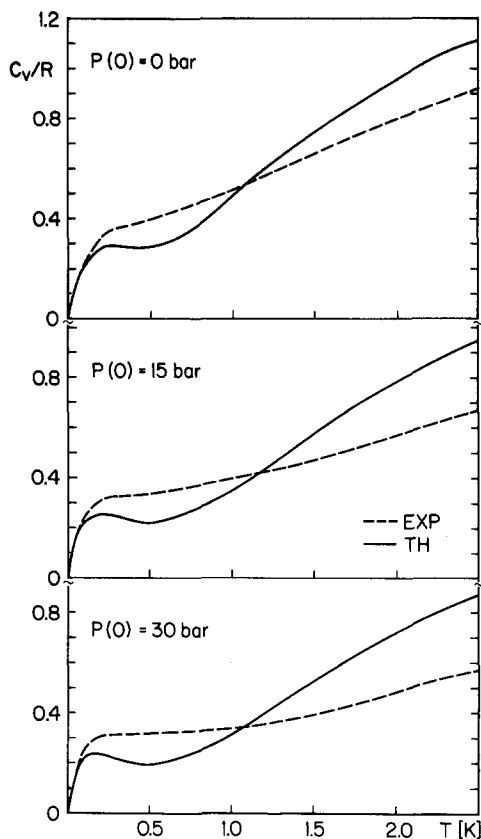


Fig. 2. Temperature dependence of c_v of normal ${}^3\text{He}$ below 2.5 K for the three molar volumes 36.84, 28.86, and 26.14 cm^3 that correspond to the zero-temperature pressures $P(0) = 0, 15,$ and 30 bar. (--) Experiment (Greywall⁶); (—) theory.

It is also interesting to plot (Fig. 3) the results as c_v/T versus T . These plots clearly show that the derivations from a linear specific heat set in at temperatures $T \ll T_F^*$. This is a reflection of the bound on the spin entropy, which causes the spin contribution to the specific heat to peak well before the entropy saturates at T_F^* . (See also ref. 10.) A similar effect is seen if one calculates the specific heat of noninteracting fermions in a half-filled band with finite width, where the peak in the specific heat is a factor of 5 below the Fermi temperature. Returning to the comparison of theory and experiment for $c_v(T)$, we see a slight peak in the total specific heat from this effect, which in the experiment appears as a sharp turnover into a

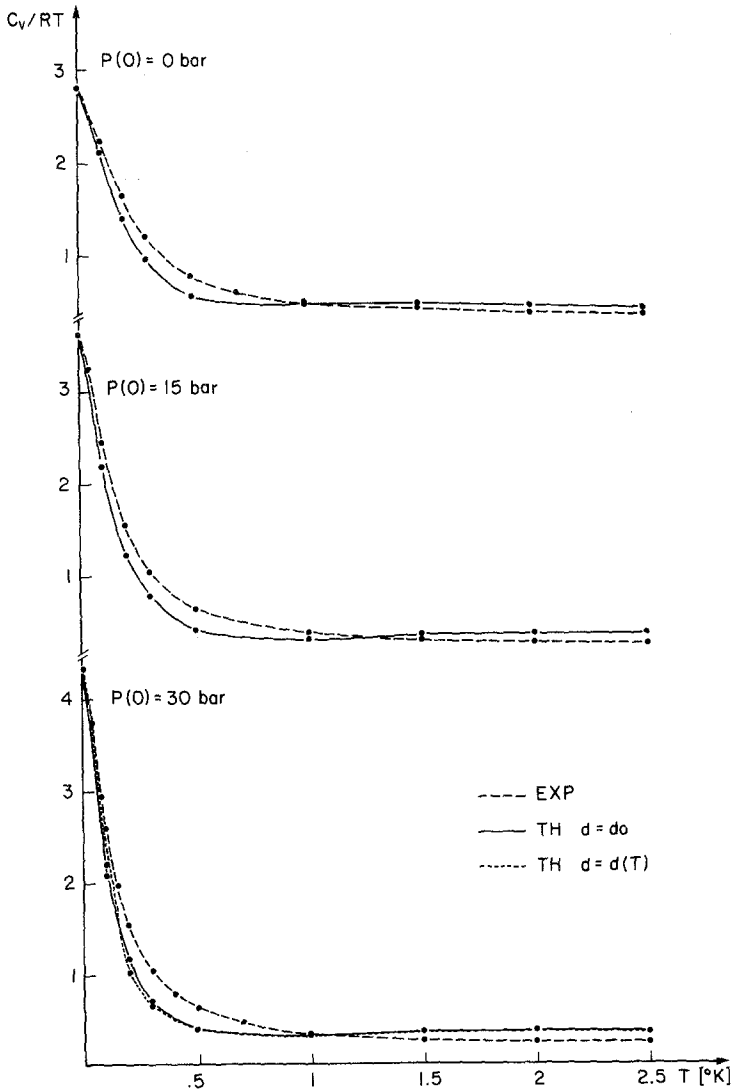


Fig. 3. Temperature dependence of c_v/T of normal ^3He below 2.5 K for the three molar volumes 36.84, 28.86, and 26.14 cm^3 that corresponds to the zero-temperature pressures $P(0) = 0, 15,$ and 30 bar. For $V = 26.14 \text{ cm}^3$ [$P(0) = 30 \text{ bar}$] we also show the result where all the parameters are calculated self-consistently. Note the very narrow regime of constant c_v/T . (---) Experiment (Greywall⁶); (—) theory ($d = \text{const}$); ($\cdot\cdot\cdot$) theory [$d = d(T)$].

plateau. Clearly this peak is an artifact of our oversimplified treatment of the high-energy states.

Greywall⁶ recognizes that the family of curves $[c_v(P) - c_v(0)]/c_v(0)$ for different molar volumes had the peculiar property that they all intersect at a single temperature of ~ 160 mK. We have made a corresponding plot of our results in Fig. 4. Although the curves do not intersect in a single point, the overall features of the experiment are reproduced.

For completeness we show the entropy curves in Fig. 5. One can see the tendency of the entropy to saturate at the value $R \ln 2$ at low temperatures. Above about 0.5 K the contribution of the free states becomes more and more important and the entropy again rises.

As mentioned before, these calculations were done using the zero-temperature values of A , R , and d . To check the validity of this assumption, the system of equations $\partial F/\partial d = 0$, particle conservation, and the two sum rules (10) and (12) was solved self-consistently for A , R , and d as functions of T at $P = 30$ bar. Figure 6 shows the results for $d(T)$. As temperature is increased, $d(T)$ drops initially, i.e., the system has the tendency to localize even further to maximize the entropy. A little bit below $T = 0.2$ K there is a sharp minimum. Afterwards d increases and when $T \gg T_F^*$ it approaches the asymptotic form (11). The effect of this temperature dependence of A , R , and d on the specific heat and on the entropy is not large, as can be

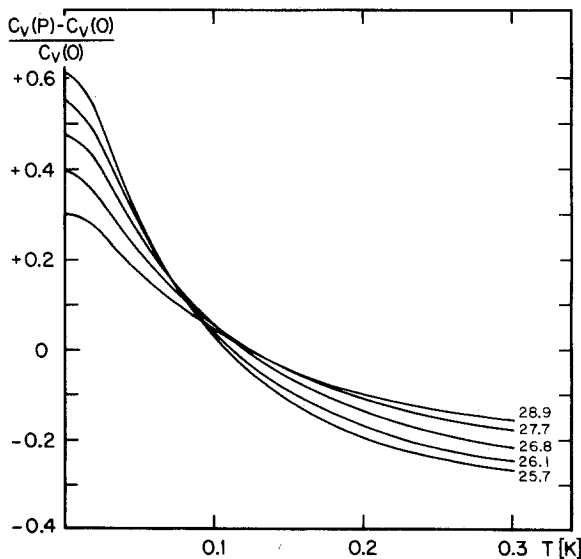


Fig. 4. The calculated family of curves $[c_v(P) - c_v(0)]/c_v(0)$ as functions of T at different molar volumes in cm^3 .

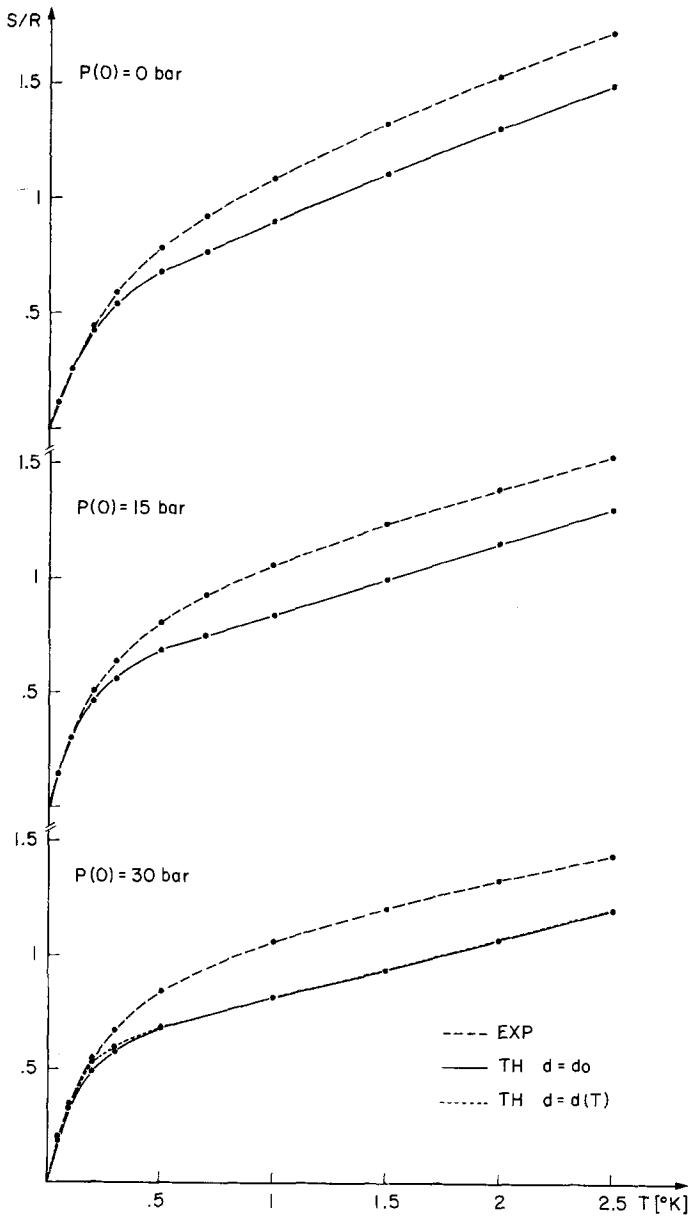


Fig. 5. Temperature dependence of the entropy of normal ^3He . One can see the tendency of the entropy of the correlated states to saturate at the value $S = R \ln 2$. For higher temperatures the entropy again rises due to the free states. (---) Experiment (Greywall⁶); (—) theory ($d = \text{const}$); (···) theory [$d = d(T)$].

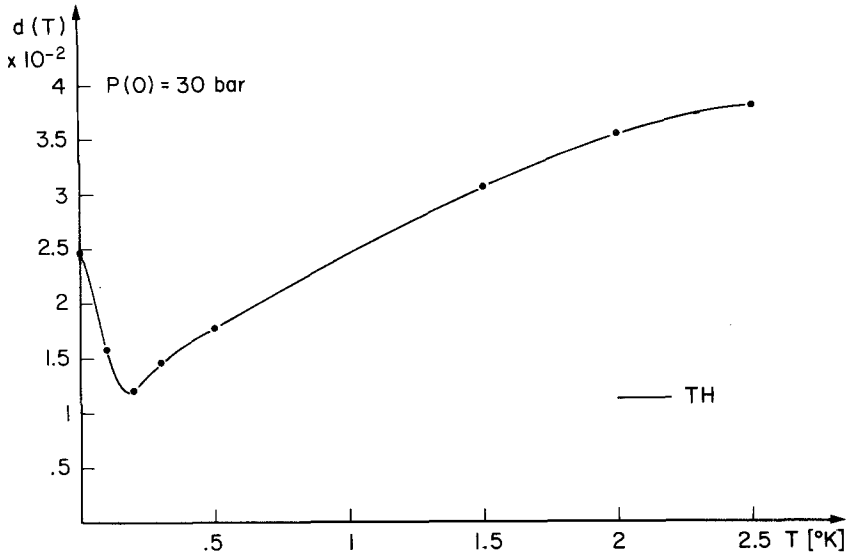


Fig. 6. Temperature dependence of the concentration of doubly occupied sites d , for $V = 26.14 \text{ cm}^3$ [$P(0) = 30 \text{ bar}$].

seen in the $P = 30 \text{ bar}$ results (Figs. 3 and 5). Therefore we have used the simplifying approximation $d(T) = d(0)$ for the other pressures.

5. THE SPIN SUSCEPTIBILITY

To calculate the spin susceptibility we start from the formula

$$\mu_0^2 \chi_s^{-1} = \left. \frac{\partial^2 F}{\partial m^2} \right|_{m=0}$$

One gets at once from (6)

$$\begin{aligned} \mu_0^2 (\chi_s^c)^{-1} = & \sum_{\sigma} \frac{\partial^2 q_{\sigma}}{\partial m^2} \sum_{\mathbf{k}} n_{\mathbf{k}\sigma} \varepsilon_{\mathbf{k}} + \frac{1}{2} \sum_{\sigma} \sigma \frac{\partial q_{\sigma}}{\partial m} \mu_{\sigma} \\ & - T^{-1} \sum_{\sigma} \left(\frac{\partial q_{\sigma}}{\partial m} \right)^2 \sum_{\mathbf{k}} n_{\mathbf{k}\sigma} (1 - n_{\mathbf{k}\sigma}) \varepsilon_{\mathbf{k}} \frac{\varepsilon_{\mathbf{k}} - \mu_{\sigma}}{w_{\mathbf{k}}} \\ & + T^{-1} \sum_{\sigma} \frac{\partial q_{\sigma}}{\partial m} q_{\sigma} \frac{\partial \mu_{\sigma}}{\partial m} \sum_{\mathbf{k}} \varepsilon_{\mathbf{k}} n_{\mathbf{k}\sigma} \frac{1 - n_{\mathbf{k}\sigma}}{w_{\mathbf{k}}} + \frac{1}{2} \sum_{\sigma} \sigma q_{\sigma} \frac{\partial \mu_{\sigma}}{\partial m} \end{aligned} \quad (23)$$

Writing

$$n = \sum_{\sigma} \sum_{\mathbf{k}} n_{\mathbf{k}\sigma}, \quad m = \sum_{\sigma} \sum_{\mathbf{k}} \sigma n_{\mathbf{k}\sigma}$$

we can calculate the derivative of μ_σ with respect to m from the two relations $\partial m/\partial m = 1$, $\partial n/\partial m = 0$. The result is

$$\frac{\partial \mu_\sigma}{\partial m} = \frac{\sigma/2 + (\partial q_\sigma/\partial m) \sum_{\mathbf{k}} n_{\mathbf{k}\sigma} (1 - n_{\mathbf{k}\sigma}) (\varepsilon_{\mathbf{k}} - \mu_\sigma) / Tw_{\mathbf{k}}}{q_\sigma \sum_{\mathbf{k}} n_{\mathbf{k}\sigma} (1 - n_{\mathbf{k}\sigma}) / Tw_{\mathbf{k}}} \quad (24)$$

Inserting (24) into (23) yields

$$\begin{aligned} \mu_0^2(\chi_s^c)^{-1} &= \frac{\partial^2 q}{\partial m^2} I_3^c + 2 \left| \frac{\partial q}{\partial m} \right| \frac{I_5^c}{I_2^c} \\ &\quad + \left(\frac{\partial q}{\partial m} \right)^2 \left[\frac{(I_5^c)^2}{I_2^c} - I_4^c \right] + \frac{1}{I_2^c} \end{aligned} \quad (25)$$

Here

$$I_3^c = \int dE N_c(E) n(E - \mu) (E - 1) \quad (26)$$

$$I_4^c = \int dE N_c(E) n(E - \mu) [1 - n(E - \mu)] (E - 1)^2 / [Tw(E)] \quad (27)$$

$$I_5^c = \int dE N_c(E) n(E - \mu) [1 - n(E - \mu)] (E - 1) / [Tw(E)] \quad (28)$$

I_2^c has already been defined in (21). The term with $(\partial q/\partial m)^2$ can be shown to be proportional to δ^2 and can thus be neglected. Therefore our final result is

$$\mu_0^2(\chi_s^c)^{-1} = \frac{\partial^2 q}{\partial m^2} I_3^c + 2 \left| \frac{\partial q}{\partial m} \right| \frac{I_5^c}{I_2^c} + \frac{1}{I_2^c} \quad (29)$$

The explicit expressions for the derivatives of q with respect to m can be obtained from (3). In the limit $T=0$ one obtains for the Wilson ratio

$$\frac{\chi_s/\chi_0}{m^*/m} = \left\{ 1 - p \left[1 - \frac{1}{(2-4d)^2} \right] \right\}^{-1} \quad (30)$$

in agreement with the result of Vollhardt² [$\chi_0 = N(E_F)\mu_0^2$ is the bare susceptibility].

For intermediate temperatures $T > T_F^*$ but still $T \ll U$, $n(E - \mu) \rightarrow (1 - \delta)/2$ and therefore $I_3^c \approx I_5^c \approx 0$. We thus obtain a Curie form

$$\chi_s^c \approx \mu_0^2 \left(\sum_{\mathbf{k}} (1/w_{\mathbf{k}}) \right) / 2T \quad (31)$$

In this limit the number of magnetic moments should simply be given by the number of singly occupied sites. This condition is expressed in the sum rule (12).

The measured and calculated susceptibilities (including a small contribution from the free part of the DOS) for the different pressures are shown in Fig. 5. In the high-pressure case also the effect of the temperature variation

of A , R , and d is displayed. We can see that our susceptibility exhibits a crossover from Pauli to Curie behavior at the renormalized Fermi temperature, as observed experimentally.²¹ The overall agreement between theory and experiment is satisfactory, especially when one considers the simplicity of the model and the fact that no additional fitting parameters were introduced.

Béal-Monoc *et al.*¹¹ have derived a relation for the initial T^2 corrections to the spin susceptibility in the paramagnon theory. They showed that the T^2 coefficient is proportional to $(\chi_s/\chi_0)^2$ and found excellent agreement with the experimental results both for this form and even the magnitude of the numerical prefactor. We have made a corresponding expansion of our results and the details are given in Appendix A. We also find that the coefficient of the T^2 correction is proportional to $(\chi_s/\chi_0)^2$, or $T^2/(T_F^*)^2$ in our notation, but the numerical prefactor is considerably larger, by a factor of 8, than in the paramagnon theory. (Had we used $d = d(m, T)$ instead of $d = d_0 = \text{const.}$ for calculating χ_s , the prefactor would have only differed by a factor of 2.5.) This can be observed in Fig. 7, where the initial drop of our results is steeper than in the experiment. However, the overall shape agrees quite well with experiment. We also point out that in the susceptibility the deviations from a rescaled free fermion behavior with T_F^* instead of T_F are not too large, in contrast to the specific heat or entropy and the thermal expansion to be discussed below. The relation of the T -dependence of χ_s to the magnetization dependence of the specific heat is discussed in Appendix B.

Finally we make some remarks about the relationship between the temperature dependence between the entropy and the susceptibility. In Goldstein's approach¹⁰ the molar entropy S is

$$S = (T/\mu_0^2)\chi_s R \ln 2 \quad (32)$$

From Fermi liquid theory we know that, as $T \rightarrow 0$,

$$S = R \frac{\pi^2}{2T_F^*} T; \quad \chi_s = \mu_0^2 N(E_F) \frac{m^*/m}{1 + F_0^a} \quad (33)$$

For (32) to be correct in the limit $T \rightarrow 0$ we need to have

$$(1 + F_0^a)^{-1} = \pi^2/(3 \ln 2)$$

This yields a value $F_0^a = -0.79$, which is rather close to the experimentally found value of $0.76 \leq F_0^a \leq 0.70$! We remark that a recent result by Castaing²² presents an interesting analogy to this finding. He showed that if there existed a random internal field acting on the spins whose distribution had a constant density near zero field, then F_0^a should tend toward a limiting value of $F_0^a = -0.75$ as the solid is approached. In the almost localized model one obtains $F_0^a = -\frac{3}{4}p$, $p \approx 1$.

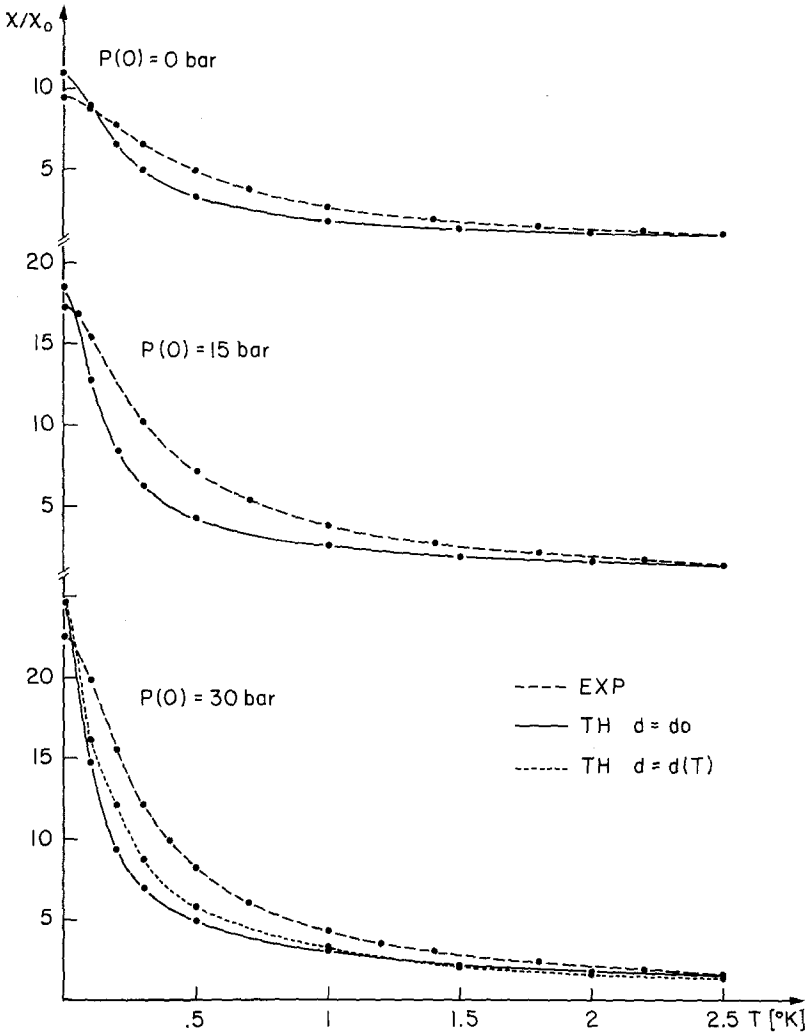


Fig. 7. Temperature dependence of the spin susceptibility of normal ^3He below 2.5 K. (---) Experiment (Ramm *et al.*²¹); (—) theory ($d = \text{const}$); (-·-) theory [$d = d(T)$].

6. THE TEMPERATURE DEPENDENCE OF THE PRESSURE AT CONSTANT VOLUME

The thermal expansion of ^3He at low temperature is anomalous; i.e., for $T \lesssim 1$ K there is actually a thermal contraction. At higher temperatures there is, as usual, a thermal expansion. The explanation of this unusual behavior is clearly a challenge to any theory of the thermodynamic properties

of ^3He . In his recent comprehensive series of experiments, Greywall⁶ presented data on the temperature dependence of the pressure at constant volume rather than the thermal expansion per se and we will therefore calculate the former and compare our results with his experiments.

An anomalous thermal expansion α at low temperatures has been found theoretically by Goldstein²³; his result $\alpha \propto \kappa(T)c_v(T)$, where κ is the compressibility, is equivalent to assuming that the Grüneisen parameter remains temperature independent up to and through the plateau region in $c_v(T)$. A qualitatively similar result for α has been obtained²⁴ using the Brueckner–Gammel theory.

We should say at once that the almost localized fermion model is a model only for the low-lying excited states of ^3He and is not meant, nor can it be used as, a model for all the ground-state properties. Thus, we will not discuss the pressure–volume relationship at $T=0$ K, which involves a consideration of the interatomic potential. Instead, we will discuss only the changes in pressure as T increases, since these reflect the nature of the low-energy excited states. The key parameter is the pressure dependence of the d parameter, which controls the specific heat. This we take simply from the value of d obtained from the volume-dependent linear specific heat coefficient. Since the thermodynamic properties are not very sensitive to the detailed shape of the w -function so long as the sum rules are satisfied, we neglect the volume dependence of A and R parameters.

From the expression for the free energy F , it is straightforward to calculate the pressure

$$P(T) = -(\partial F / \partial V)|_{T,N} \quad (34)$$

The effective mass parameter q has a volume dependence given by

$$\frac{\partial q}{\partial V} = \frac{2}{1-\delta^2} \left\{ 2(1-2\delta-4d) + 4[d(d+\delta)]^{1/2} + \frac{(1-\delta-2d)(2d+\delta)}{[d(d+\delta)]^{1/2}} \right\} \frac{\partial d}{\partial V}$$

where we have also neglected the small corrections from any volume dependence of δ . Table I gives the values of $\partial d / \partial (\ln V)$ obtained by fitting to the experimental linear coefficient of the specific heat at various volumes. Lastly, the volume derivative of μ , the chemical potential, is calculated from the particle conservation condition (18).

The results are shown in Fig. 8. In the limit $T \rightarrow 0$ the entropy is linear and $S(T) = R(\pi^2/2)(T/qT_F)$. Using the relationship $(\partial P / \partial T)_{V,N} = (\partial S / \partial V)_{T,N}$, we get the limiting form of $[P(T) - P(0)]_{V,N}$ as

$$P(T) - P(0) = n \left(\frac{\pi}{2} \right)^2 \frac{T^2}{T_F^3} \left(\frac{2}{3} - \frac{\partial \ln q}{\partial \ln V} \right) \quad (35)$$

where n is the density of particles.

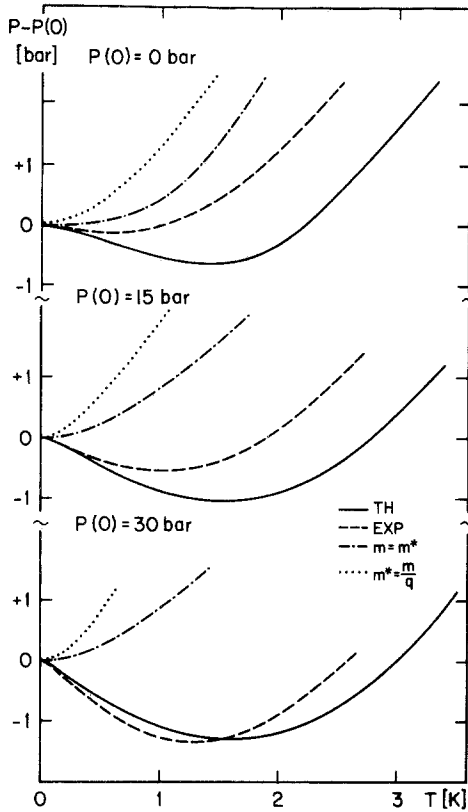


Fig. 8. Variation of the pressure as a function of temperature. Besides the theoretical (—) and experimental⁶ (---) curves, the results for free fermions ($m^* = m$) and for free fermions with rescaled mass ($m^* = m/q$) are also shown.

The volume dependence of q overwhelms the free fermion contribution and is responsible for the thermal contraction as $T \rightarrow 0$. This strong volume dependence originates in the increase in the model of U toward U_c , the critical value. At higher temperatures the spin contribution to the entropy $S(T)$ saturates at a value $\sim R \ln 2$ independent of the volume, and therefore at higher temperatures the free fermion behavior dominates. The result is a minimum in $[P(T) - P(0)]_{V,N}$, in contrast to the behavior of free fermions. In Fig. 8 we see that the position and depth of the minimum are reproduced reasonably well by the model. At the smallest molar volume ($v = 26.14 \text{ cm}^3$) the agreement is better than 1% in P up to $T = 2 \text{ K}$. While we expect better

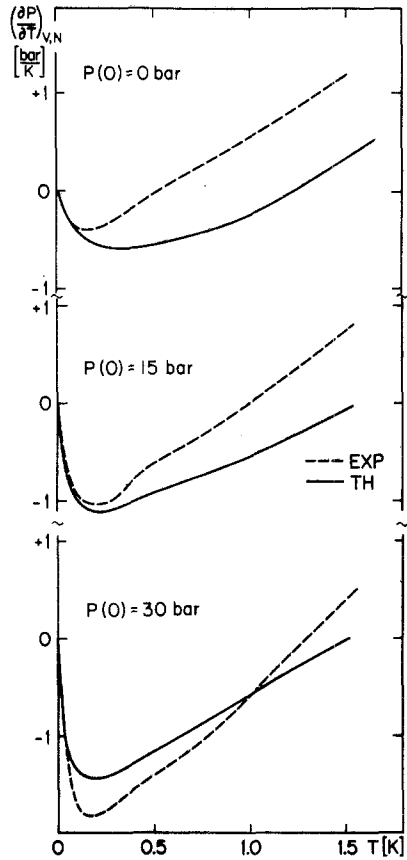


Fig. 9. The calculated $(dP/dT)|_{V,N}$ versus T at different molar volumes 36.84, 28.86, and 26.14 cm^3 that corresponds to the zero-temperature pressures 0, 15, and 30 bar. (--) Experiment (Greywall⁶); (—) Theory.

agreement as $U \rightarrow U_c$, such excellent agreement is somewhat fortuitous for our simple model.

In Fig. 9 we show $(dP/dT)|_{V,N}$ versus T at various molar volumes. Greywall noticed from his experimental data that the minima of these curves all occurred at the same temperature, namely where the thermal expansion coefficient is zero, and where the family of curves $[c_v(P) - c_v(0)]/c_v(0)$ intersect. We see that this feature is well reproduced by our results.

7. CONCLUSIONS

In this paper we have presented an extension of the model of almost localized fermions to finite temperature. This extension was made in a

phenomenological way, but with the use of a number of simple and physical constraints. It was achieved without the introduction of additional parameters. The model was tested by comparing three different thermodynamic properties, specific heat (or, equivalently, entropy), spin susceptibility, and the temperature-dependent pressure (or, equivalently, the thermal expansion). An acceptable fit was found simultaneously for all three properties throughout the region that covers the crossover from Landau Fermi liquid behavior to classical statistics. In the almost localized fermion model as a whole there is essentially only one free parameter in the model Hubbard Hamiltonian, which is used to describe the low-energy excitations. We regard the ability to describe so much with just one free parameter as a decided success for the almost localized model. The weakest point of the model is undoubtedly the description of the higher energy states as simply free states and the abrupt change from strongly correlated to free behavior. This was chosen so as to preserve the simplicity of the model, but improvements could be made here. Another desirable direction would be the extension to cover the actual dynamics of ^3He , but that requires further consideration and is outside the scope of this paper. Finally, we believe that the successful description of so much data through this simple model is further confirmation of the dominant role of local spin fluctuations in the low-energy excitation spectrum and of the overall physical description of ^3He as an almost localized or almost crystalline liquid.

APPENDIX A: LOW-TEMPERATURE EXPANSION OF THE SPIN SUSCEPTIBILITY

We want to expand in powers of T integrals of the type

$$\begin{aligned} J &= \int_{1-\Delta}^{1+\Delta} d\varepsilon H_c(\varepsilon) n_c(\varepsilon - \mu) + \int_{E_c}^{\infty} d\varepsilon H_f(\varepsilon) f(\varepsilon - \mu) \\ &= \int_{-\infty}^{\infty} d\varepsilon H_c(\varepsilon) n_c(\varepsilon - \mu) + O(e^{-q\Delta/T}) \end{aligned} \quad (\text{A1})$$

where energies are measured in units of E_F and with

$$\begin{aligned} n_c(\varepsilon - \mu) &= 1 / \{1 + \exp[q(\varepsilon - \mu) / w(\varepsilon) T]\} \\ w(\varepsilon) &= B + A \exp[-(\varepsilon - 1)^2 / R^2] \end{aligned}$$

The method is insensitive to $H(\varepsilon)$ as long as $H(\varepsilon)$ goes to zero fast enough for $\varepsilon \rightarrow -\infty$.

We define

$$F_H(\varepsilon) = \int_{-\infty}^{\varepsilon} d\varepsilon' H(\varepsilon') \quad (\text{A2})$$

Partial integration of (A1) yields

$$J = \int_{-\infty}^{\infty} d\varepsilon F_H(\varepsilon) n_c(\varepsilon - \mu) [1 - n_c(\varepsilon - \mu)] \frac{\partial}{\partial \varepsilon} \left(\frac{q(\varepsilon - \mu)}{w(\varepsilon)T} \right) \quad (\text{A3})$$

As usual we expand $F_H(\varepsilon)$ around μ :

$$F_H(\varepsilon) = F_H(\mu) + H(\mu)(\varepsilon - \mu) + \frac{1}{2}H'(\mu)(\varepsilon - \mu)^2 + O[(\varepsilon - \mu)^3] \quad (\text{A4})$$

With a change of variables

$$Y = \frac{q(\varepsilon - \mu)}{Tw(\varepsilon)}, \quad dY = \frac{\partial}{\partial \varepsilon} \left(\frac{q(\varepsilon - \mu)}{w(\varepsilon)T} \right) d\varepsilon \quad (\text{A5})$$

we rewrite (A3):

$$J = \int_{-\infty}^{\infty} dY n_c(Y) [1 - n_c(Y)] \left\{ \sum_{l=0}^{\infty} \frac{Y^l}{l!} \frac{\partial^l F_H}{\partial \varepsilon^l} \Big|_{\varepsilon=\mu} \left(\frac{wT}{q} \right)^l \right\} \quad (\text{A6})$$

One can show that $w(\varepsilon) = 1 + O(T^2)$. Since we are only interested in terms up to $\sim T^2$, we can take $w(\varepsilon) \equiv 1$ in (A6). So we have a standard expression:

$$J = \int_{-\infty}^{\mu} d\varepsilon' H(\varepsilon') + (\pi^2/6) \{ H'(\mu) [1 - 2(A/R^2)(1 - \mu)^2] + 4(1 - \mu)(A/R^2)H(\mu) \} (T/T_F^*)^2 + O[(T/T_F^*)^3] \quad (\text{A7})$$

where T is now measured in Kelvins. We see that, to $O(T^{-3})$, J is independent of A , B , R , i.e., w .

Using the DOS $N_c(\varepsilon)$ for $H(\varepsilon)$ leads to an expansion for the chemical potential as ($N(0) = 3/2E_F$)

$$\mu(T) = 1 - \frac{1}{3}(\pi^2/2)^2 (T/T_F^*)^2 + O[(T/T_F^*)^3] \quad (\text{A8})$$

and taking $\varepsilon N_c(\varepsilon)$ for $H(\varepsilon)$ gives the specific heat

$$c_v(T) = R(\pi^2/2)(T/T_F^*) + O[(T/T_F^*)^3] \quad (\text{A9})$$

The formula for the spin susceptibility (23) does not have the form (A1), but a very similar one. The same procedure can be applied. The main difference in the result is that the T^2 term now depends also on A and R . We quote here only the result for $d = d_0 = \text{const.}$:

$$\frac{\chi(T)}{\chi(T=0)} = 1 - \frac{\pi^2}{6} \left(\frac{T}{T_F^*} \right)^2 \frac{\frac{9}{2} \{ 1 - [1/(1+I)]^2 \} + 4A/R^2 - p'' + (p')^2}{1 - p \{ 1 - [1/(1+I)]^2 \}} \quad (\text{A10})$$

with

$$I = u/8|\bar{\varepsilon}_0|, \quad p = 2N_c(0)|\bar{\varepsilon}_0| \\ p' = \varepsilon_F N_c'(0)/N_c(0), \quad p'' = E_F^2 N_c''(0)/N_c(0)$$

We will use the half-ellipse DOS, which has $p = 32/3\pi^2$, $p' = 0$, and $p'' = -9\pi^2/64$. For the localized limit $I = 1$ we get

$$\frac{\chi(T)}{\chi(T=0)} = 1 - \frac{\pi^2}{12} \left(\frac{T}{T_F}\right)^2 \left(\frac{4}{q}\right)^2 1.6 \left(1.4 + 1.6 \frac{A}{R^2}\right) \quad (\text{A11})$$

We want to compare this result with paramagnon theory,¹¹

$$\frac{\chi_{\text{paramagnon}}}{\chi(T=0)} = 1 - \frac{\pi^2}{12} \left(\frac{T}{T_F}\right)^2 \frac{1.6}{K_0^4} \quad (\text{A12})$$

where $1/K_0^2 = \chi(T=0)/\chi_0$, which tends to $4/q$ for the localized limit. The enhancement of the quadratic T -term relative to the free fermion value is $1.6/K_0^4$. The paramagnon result (A12) agrees well with experiment.^{21,25} With $A = 0.78$ and $R = 0.44$ our T^2 term is a factor 8 too large, but it also scales with $1/K_0^4$. (Note that if we had used the full $d(m, T)$ instead of $d = d_0 = \text{const.}$ for the calculation of χ_s , the T^2 -term would have only differed by a factor of 2.5.) Since our overall results are quite good, the higher terms in the expansion soon compensate the T^2 term.

APPENDIX B: THE MAGNETIZATION DEPENDENCE OF THE SPECIFIC HEAT

In Section VI.D. of ref. 2 the magnetization dependence of q^{-1} (the inverse of the discontinuity at the Fermi surface at $T=0$) was calculated. At $T=0$ and magnetization $m=0$ one has $m^*/m = q^{-1}$ and hence the result was taken as a calculation of the m -dependence of the effective mass m^* itself. It was found that in the range of interaction strengths valid for ^3He , q^{-1} and hence m^* increased for increasing magnetization.

Assuming that this $T=0$ result could be used to determine the linear specific heat coefficient γ , Quader and Bedell²⁶ pointed out that it would conflict with the behavior deduced from the temperature dependence of the susceptibility $\chi_s(T)$. (Note, however, that these authors did not consider the reduction of the density of states due to the magnetic field when they related the results of ref. 2 for m^*/m to γ). Indeed, γ and χ_s can be calculated from the free energy F as

$$\gamma = - \left. \frac{\partial^2 F}{\partial T^2} \right|_{T=0}, \quad \frac{\mu_0^2}{\chi_s} = \left. \frac{\partial^2 F}{\partial m^2} \right|_{m=0} \quad (\text{B1})$$

and must obey the Maxwell relation $\mu_0 \partial m / \partial T = \partial S / \partial H$ which, for a Fermi liquid, may be written as¹¹

$$\frac{1}{H} \left. \frac{\partial \gamma}{\partial H} \right|_{H=0} = \left. \frac{\partial^2 \chi_s}{\partial T^2} \right|_{T=0} \quad (\text{B2})$$

This relation follows from the fact that $F(m, T)$ may be expanded in a power series for small m and T and that the mixed term ($\alpha m^2 T^2$) determines,

via (B1), both sides of (B2). Clearly we may use such an expansion of our free energy F in (5). If the magnetization dependence of q^{-1} obtained in ref. 2 did apply to γ , it would follow that for $P \geq 16$ bar $\partial^2 \gamma / \partial m^2 > 0$, which is in conflict with the experiment via (B2) since, experimentally $\partial^2 \chi_s / \partial T^2|_{m, T=0} < 0$. Furthermore, the results of the present paper, which do satisfy (B2), give $\partial^2 \chi_s / \partial T^2 > 0$ at all pressures. It remains to explain the origin of this discrepancy.

The expansion of $F(m, T)$ yields the following expression for γ

$$\gamma = -2 \left\{ \left. \frac{\partial F}{\partial T^2} \right|_{m=0, T=0} + \frac{\partial}{\partial T^2} \left[\left. \frac{\partial F}{\partial m^2} + \frac{\partial F}{\partial d} \frac{\partial d}{\partial m^2} \right] \right|_{m=0, T=0} m^2 \right\} \quad (\text{B3})$$

$$= \frac{\gamma_0}{q_0} \left\{ 1 + m^2 \left[\frac{2}{9} \left(p'' - \frac{4A}{R^2} \right) - Q \right] \right\} \quad (\text{B4})$$

with $\gamma_0 = (\pi^2/3)N(0)$, $p'' = E_F^2 N''(0)$, $q_0 = 8d_0(1 - 2d_0)$; here $d_0 = d(m=0, T=0)$ and

$$Q = \frac{1}{q_0} \left. \frac{dq}{dm^2} \right|_{T=0}$$

What is of interest now is the sign of the m^2 -coefficient in (B4). The dominant contribution comes from the A/R^2 -term. As long as this term is present we always have $\partial^2 \gamma / \partial m^2 < 0$. Without it the sign of Q becomes important. Using the full m - and T -dependent d , i.e., $d = d(m, T)$, one finds

$$Q = -\frac{2I^2}{1-I^2} \left[\frac{1}{2} - \frac{1}{p} + \frac{1}{(1+I)^2} \right] \quad (\text{B5})$$

This result has already been obtained in ref. 2. In the case that d is kept constant, i.e., $d = d_0$ (an approximation used in this paper for computational convenience only), the term $\partial d / \partial T^2$ in (B3) is not present leading to

$$Q = 1 - \frac{1}{(1+I)^2} \quad (\text{B6})$$

which is always positive.

The term $4A/R^2$ in (B4) arises because we have chosen the entropy weighting function $w(E)$ as independent of the magnetization m and a function only of $E - E_F$, even for $m \neq 0$. The choice of $w(E)$ is consistent with the very weak dependence of the sum rules (9) and (12) on m . Note, that the m^2 -term of γ in (B4) (and, correspondingly, the T^2 -term in χ_s) comes from the $m^2 T^2$ -term in F . Such a term goes beyond the obvious range of applicability of Landau theory which only discusses corrections to the groundstate energy up to 2nd order in a perturbation. Since the weighting

function w only enters in higher than 2nd order, its choice (and, in particular, the choice of the energy dependence) will only affect these higher order terms. In fact, if w was chosen as a function of $E - \mu_\sigma$, the A/R^2 -term in (B4) would *not* enter (it only comes in at even higher orders of T). Such an energy dependence would correspond to a separate weighting of two, independent Fermi surfaces for up and down spins. As it leads to the same $m^2 T^2$ -term as does $w \equiv 1$ (corresponding to Landau theory) it is equivalent to assuming that this term may be calculated within the Landau theory itself. In that case (B4) reduces to the result obtained by Vollhardt,² who in fact relied on this very assumption. (This also proves that the results of ref. 2 do not violate a Maxwell relation as stated in ref. 26.) On the other hand, the correlations between the up- and down-spin particles are expected to mix the energy states in the region of k -space between the two Fermi surfaces. Then the weighting function should include all the states between $E - \mu_\uparrow$ and $E - \mu_\downarrow$, i.e., those which are centered around E_F (the Fermi energy without magnetization). This is achieved by choosing w as a function of $E - E_F$. Consequently one obtains (B4) and thus the correct sign for $\partial^2 \chi_s / \partial T^2$ at all pressures.

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