Single-Particle Spectrum and Specific Heat of Liquid ^{3}He

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The behavior of the specific heat of liquid ^{3}He, over a wide range of temperature, indicates a wiggle in the single-(quasi)particle spectrum $e(k)$ at k_F. This wiggle corresponds to the enhancement of the effective mass $m^*(k)$ at k_F of current interest in nuclear physics. It can be quantitatively understood from the microscopic Hamiltonian within correlated-basis perturbation theory.

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The specific heat of liquid ^{3}He in the millikelvin region has been mostly discussed from the point of view of low-temperature expansions. The older work has been reviewed by Baym and Pethick,[1] and a new discussion of this region, which is very closely related to the present work, may be found in a recent paper by Brown, Pethick, and Zaringhalam.[2]

Here we study the specific heat of liquid ^{3}He at equilibrium density over a much wider temperature region up to 2 K. The main feature of the measured specific heat, shown by curve $C_{ve}(T)$ in Fig. 1, is a sharp bend at ~0.2 K. We propose that this feature is due to a wiggle in the single-(quasi)particle spectrum $e(k)$ at k_F, as shown by curve $e_s(k)$ in Fig. 2.

The effective mass $m^*(k)$ is given by the slope of $e(k)$:

$$m^*(k) = \hbar^2 k / [de(k)/dk], \tag{1}$$

and the wiggle in $e(k)$ at k_F implies a large enhancement of m^* in a narrow region around k_F. Such an enhancement of m^* at k_F was first noticed by Brown, Gunn, and Gould[3] in nuclei. It has been discussed in the framework of Brueck-

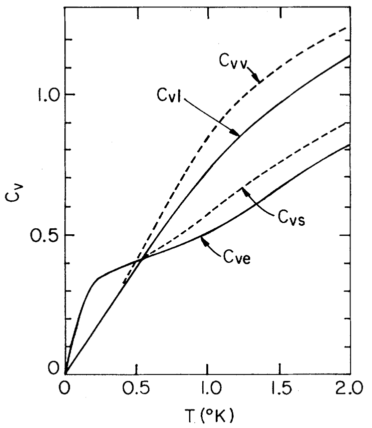

FIG. 1. The specific heat at constant volume. The curves C_{v1}, C_{vv}, and C_{vs} give results of first-order, variational, and schematic calculations, while C_{ve} gives the experimental results. $C_{vs} \approx C_{ve}$ and $C_{vv} = C_{v1}$ at small temperatures.

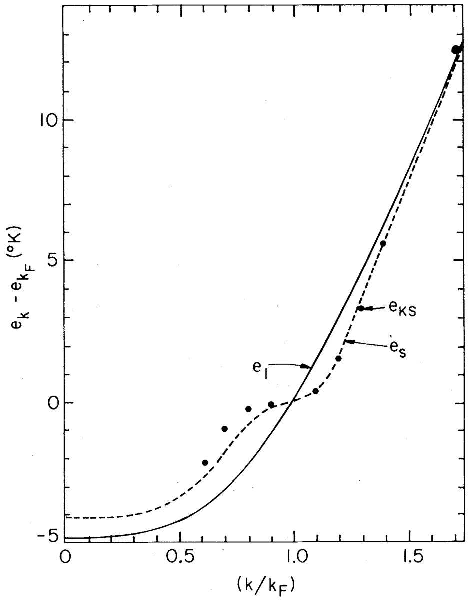

FIG. 2. The single-particle spectrum $e(k)$. The curves e_1 and e_s give results of first-order and schematic calculations, while points e_{KS} show the results of Krotscheck and Smith.

ner's theory by Jeukenne, Lejeune, and Mahaux.[4] However, the effect appears to be much more pronounced in liquid ^{3}He than in nuclear matter.

Our approach is microscopic; it uses the bare Lennard-Jones (6, 12) Hamiltonian, and the formalism of correlated-basis perturbation theory (CBPT). This theory, developed originally by Feenberg and collaborators,[5] is based on the observation that a fairly good description of the ground-state energy and distribution functions can be obtained with variational wave functions $\mathcal{G}\Phi_0$, where $\mathcal{G}$ is a correlation operator and Φ_0 the noninteracting ground state. A correlated basis Ψ_i is defined as $\mathcal{G}\Phi_i$, where Φ_i are noninteracting gas states. If $\mathcal{G}$ is not unitary, as is the case in practice, Ψ_i have to be orthogonalized. When Ψ_0 gives a good description of the ground state we can expect the Ψ_i to be close to the eigenstates of the liquid, so that perturbation theory converges in this basis.

CBPT has been recently used, with some success, to study the single-particle states of nuclear matter. The first-order spectrum[6] $e_1(k)$ is given by the energy differences $\langle E_{\mathrm{p/h}}\rangle - \langle E_0\rangle$, where $\langle E_{\mathrm{p/h}}\rangle$ are expectation values with wave functions $\mathcal{G}\Phi_{\mathrm{p/h}}$. The $\Phi_{\mathrm{p/h}}$ are states with one particle/hole excitation. The imaginary part $W(k)$ of the single-particle energy,[7] as well as corrections[8] to $e(k)$, have been calculated in second-order CBPT. Results of pedagogical models have been reported by Krotscheck, Smith, and Jackson.[9] The experimental data[6] indicate the presence of a small wiggle in $e(k)$ at k_{F}; the theoretical $e_1(k)$ does not have any structure at k_{F}; however, the second-order effects tend to produce it.

The $e_1(k)$ obtained for liquid ^{3}He at $\rho = 0.277$ atom/σ^3 ($\sigma = 2.556$ Å) is shown in Fig. 2. It is calculated by methods given in Ref. 6, and chain summation methods[10] are used to calculate $\langle E_{\mathrm{p/h}}\rangle$ and $\langle E_0\rangle$. The correlation operator $\mathcal{G}$ of Ref. 10 is used. It contains two-body, three-body, and momentum-dependent (back-flow) correlations:

$$\mathcal{G} = \prod_{i<j} f_J(r_{ij}) \prod_{i<j<k} f_3(\vec{\mathrm{r}}_{ij}, \vec{\mathrm{r}}_{ik}) \prod_{i<j} [1 + i f_K(r_{ij}) \vec{\mathrm{r}}_{ij} \cdot (\vec{\mathrm{k}}_i - \vec{\mathrm{k}}_j)], \tag{2}$$

and $f_J(r_{ij})$, $f_3(\vec{\mathrm{r}}_{ij}, \vec{\mathrm{r}}_{ik})$, and $f_K(r_{ij})$ are variational functions.[10] The E_0 obtained with this $\mathcal{G}$ by chain summation methods[10] is -1.9 K (per particle). Monte Carlo calculations[11] with a similar $\mathcal{G}$ give -1.7 K. From available Green's-function Monte Carlo calculations[12] and results given in Ref. 11 we surmise that the correct ground-state energy for the Lennard-Jones Hamiltonian is ~ -2 K. The experimental E_0 is -2.47 K; the difference is attributed to deficiencies of the Lennard-Jones potential.

The first-order $e_1(k)$ can be thought of as the Hartree-Fock spectrum in the correlated basis. The effective mass $m_1^*(k_{\mathrm{F}})$ is $0.76m$, certainly too small by a factor of 3 to 4. The $m^*(k_{\mathrm{F}})$ obtained from the experimental specific heat at very low temperatures is much larger ($2.2m$ and $2.9m$ according to Alvesalo *et al.*[13] and Mota *et al.*,[14] respectively). However, the following calculations indicate that the $e_1(k)$ at large values of $|k - k_{\mathrm{F}}|$ is satisfactory.

In the simplest approximation the thermal properties may be calculated from the $e_1(k)$ at $T = 0$. We use units in which the Boltzmann constant is 1, so that the entropy S and specific heat C_v (per particle) are dimensionless. The entropy $S(T)$ is given by

$$S(T) = (-3/k_{\mathrm{F}}^3) \int k^2\, dk [(1 - n_k)\ln(1 - n_k) + n_k \ln n_k], \tag{3}$$

$$n_k(T) = 1/\{\exp[(e(k) - \mu)/T] + 1\}. \tag{4}$$

The free energy $F(T)$ and $C_v(T)$ are given by

$$\partial F(T)/\partial T = -S(T), \tag{5}$$

$$C_v(T) = T\, \partial S(T)/\partial T. \tag{6}$$

The results obtained with $e_1(k)$ are shown in Figs. 1, 3, and 4 by curves $C_{v1}(T)$, $S_1(T)$, and $F_1(T)$.

The effect of the possible temperature dependence of $e_1(k)$ is studied using the variational method at finite temperatures.[15] In this method $F(T) = \langle H\rangle_{TD} - TS$ is obtained by calculating the thermodynamic expected value $\langle H\rangle_{TD}$ directly by chain summation methods. The free energy $F(T)$ is minimized with respect to variations in $e(k)$ at every temperature. $S_v(T)$ and $C_{vv}(T)$ are obtained by differentiating $F(T)$. The results of this calculation are shown by curves S_v, F_v, and C_{vv} in the figures. We note that this variational calculation is of first order in CBPT; it is analogous to Hartree-Fock at finite temperature. The similarity of F_1, S_1, and C_{v1} with F_v, S_v, and C_{vv} suggests that $e_1(k)$ is not very temperature dependent at $T < 2$ K.

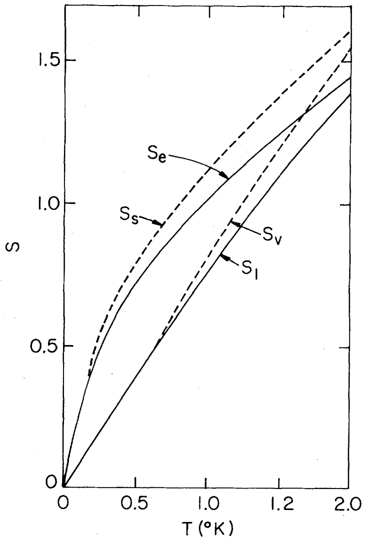

FIG. 3. The entropy per particle. The curves S_1, S_v, and S_s give results of first-order, variational, and schematic calculations, while S_e gives experimental results.

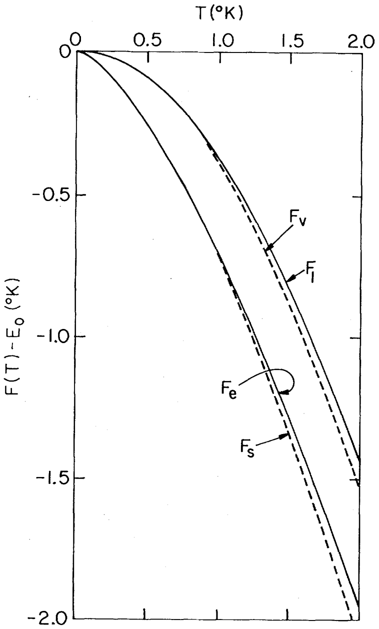

FIG. 4. The free-energy per particle. The curves F_1, F_v, and F_s give results of first-order, variational, and schematic calculations, while F_e gives experimental results.

The curves S_e, F_e, and C_{ve} give the experimental results. C_{ve} is obtained from the data of Roberts *et al.*[16] and Brewer, Daunt, and Sreedhar[17] as tabulated by Wilks.[18] The $V(P, T)$ data of Sherman and Edeskuty,[19] corrected by Wilks,[18] are used to convert the C_{sat} to C_v. Note that these data extend only above 0.12 K; we extrapolate them crudely to $C_v = 0$ at $T = 0$. The differences between the two measurements[13,14] of C_v in the millikelvin range would not be noticeable in Fig. 1.

The relative difference between the first-order quantities S_1, F_1, and C_{v1}, and the experimental S_e, F_e, and C_{ve} becomes smaller as T increases. This can be understood by taking $e(k) = \hbar^2k^2/2m^*(T)$ in Eqs. (3) and (4), and solving for the value of $m^*(T)$ necessary to reproduce the "experimental" entropy $S_e(T)$. This $m^*(T)$ decreases rapidly with T and approaches ~$0.8m$ at $T = 2$ K. Thus $m_1^*(k)$ gives the average value of m^* over a wide range around k_F.

The second-order CBPT contribution to $e(k)$ has two terms containing matrix elements $\langle p|H \times |p_1p_2h_1\rangle$ and $\langle \rho|H|pp_1h_1h_2\rangle$ for $k = p > k_F$, and $\langle h|H \times |h_1h_2p_1\rangle$ and $\langle \rho|H|hh_1p_1p_2\rangle$ for $k = h < k_F$. Here $|\,\rangle$ represent orthogonalized correlated states having the prescribed particles and holes, and a sum over p_1, p_2, h_1, and h_2 is implied. At $k = k_F$ the contributions of these two terms cancel substantially, which implies that the change in the Fermi energy $e(k_F)$ is small, as it should be since $e(k_F)$ is related to $E_0(\rho)$. However, the slopes of the contributions of these two terms add, and that changes the slope of $e(k)$ at k_F. At large $|k - k_F|$ the second-order correction becomes small compared to $|e_1(k) - e(k_F)|$, so the $e(k)$ follows $e_1(k)$ at $k \gg k_F$. The net result is a wiggle at k_F.

Here we use a schematic model of Brown and co-workers[2,20] to parametrize the contribution of higher-order CBPT terms to $e(k)$. The object is to determine the spectrum from the experimental $C_{ve}(T)$ with the assumption that $e(k)$ is not very temperature dependent. The schematic model assumes a simple energy dependence for the imaginary part $W(k, E)$:

$$E(k) = e(k) - e(k_F), \tag{7}$$

$$W(k, E) = W_0[E^2/(E^2 + E_0^2)], \tag{8}$$

and uses the dispersion integral,

$$E(k) - E_1(k) = \frac{1}{\pi}\mathrm{P}\int \frac{W(k, E')}{E(k) - E'}\,dE' = -\frac{W_0E_0E(k)}{E^2(k) + E_0^2}, \tag{9}$$

to calculate $e(k)$. The parameters W_0 and E_0 are varied to fit $C_{ve}(T)$. The $e(k)$ obtained with W_0

$= 3.08$ K and $E_0 = 1.1$ K is shown by the curve $e_s(k)$ in Fig. 2. It gives a fair description of the observed thermal properties; curves $C_{vs}(T)$, $S_s(T)$, and $F_s(T)$ show results obtained with $e_s(k)$. Brown, Pethick, and Zaringhalam[2] have estimated values of E_0 and W_0 with Landau's theory. Their values, $E_0 \sim 1$ K and $W_0 \sim 2E_0$, are quite close to what we need to explain $C_{ve}(T)$. The $C_{ve}(T < 0.2\ \mathrm{K})$ samples states having $|E(k)| \lesssim 0.5$ K. These have a large effective mass; $m^*(k_F) = 2.9m$ for $e_s(k)$. And so the $C(T < 0.2\ \mathrm{K})$ behaves crudely as that of a Fermi gas with a large m^*. At $T > 0.2$ K states having $|E(k)| > 0.5$ K contribute; they have $m^* < 1$ and cut off the rise of C_v with T, thus producing the bend in $C_v(T)$.

We also note that

(i) C_v at small temperatures[17] increases with ρ, while at higher temperature[19] it decreases with ρ, and thus the bend in $C_v(T)$ becomes sharper with ρ. We should thus expect $m_1^*(k_F)$ to decrease with ρ, while $m^*(k_F)$ increases due to the wiggle becoming more sharp.

(ii) Krotscheck and Smith[21] have calculated $e(k)$ in the Jastrow basis [obtained by neglecting f_3 and f_K in $\mathcal{G}$ of Eq. (2)], including first-, second-, and third-order-ring terms. Their results, made available to us after conclusion of this work and shown in Fig. 2, are quite close to $e_s(k)$.

(iii) It should be possible to calculate the temperature dependence of the second-order CBPT contribution to $e(k)$. We can expect the wiggle it produces to disappear at high T.

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