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Mechanism of the anomalous increase of the specific heat of helium II near the λ point

Pao Lu and P. Suebka*
Department of Physics, Arizona State University, Tempe, Arizona 85287
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We report here results of calculations of the entropy and the specific heat of liquid helium II. We investigate for $T \leq 2.1$ K only. The calculated and experimental values are very close to one another. We use Brueckner and Sawada's method with several modifications. We postulate that rotons are almost-free particles except that they have hard-core interactions.

Brueckner and Sawada[1] applied the t-matrix technique to a hard-sphere, high-density boson system and calculated the energy spectrum in fair qualitative agreement with the experimental results. With the Born approximation, Parry and Ter Haar[2] included an attractive potential in the Brueckner-Sawada framework and found that the dispersion curves in the roton region no longer bend over. Lu and Chan[3] followed Parry and Ter Haar in calculating the energy spectrum by taking into account hard-core repulsions, and hence they did not use the Born approximation. They obtained an excitation spectrum which resembled the roton spectrum. Recently Suebka and Lu[4] have explained and derived the temperature dependence of the excitation energy spectrum. They have shown that their derivation is supported by the experimental evidence.

Here we want to report the use of this idea together with several stated below to derive the entropy and the specific heat. We can understand, therefore, by means of the following calculations, the values of the entropy and the specific heat as $T \to T_\lambda$.

First we note that the final-state wave function used here is of the following form:

$$\psi_k(\mathbf{r}) = \frac{1}{\sqrt{\Omega}} \sum_{l=0}^{\infty} (2l+1) i^l e^{i\delta_l} \frac{[-n_l(ka) j_l(kr) + j_l(ka) n_l(kr)] P_l(\cos\theta)}{[n_l^2(ka) + j_l^2(ka)]^{1/2}} . \quad (1)$$

As explained previously,[3,4] this radial dependence will vanish at $r=a$, the size of the hard core. We have, for the free particles,

$$\phi_k(\mathbf{r}) = \frac{1}{\sqrt{\Omega}} e^{ikr} = \frac{1}{\sqrt{\Omega}} \sum_{l=0}^{\infty} (2l+1) i^l j_l(kr) P_l(\cos\theta) . \quad (2)$$

The choice of the phase shift $e^{i\delta_l}$ with $\tan\delta_l = j_l(ka)/[-n_l(ka)]$ is very important. We will derive this immediately below. The part of the scattering from He II, of course, is zero or $f(\theta)=0$ in

$$\psi_k(\mathbf{r}) \underset{r\to\infty}{\longrightarrow} e^{ikz} + \frac{f(\theta)}{r} e^{ikr} , \quad (3)$$

since

$$R_l(r) = A_l[\cos\delta_l\, j_l(kr) + \sin\delta_l\, n_l(kr)] = \frac{1}{kr} A_l \cos\left(kr - \frac{(l+1)\pi}{2} - \delta_l\right) , \quad (4)$$

so that

$$\sum_{l=0}^{\infty} (2l+1) i^l A_l (kr)^{-1} \cos\left(kr - \frac{(l+1)\pi}{2} - \delta_l\right) P_l(\cos\theta) = r^{-1} f(\theta) e^{ikr} + \sum_{l=0}^{\infty} (2l+1) i^l (kr)^{-1} \cos\left(kr - \frac{(l+1)\pi}{2}\right) P_l(\cos\theta) . \quad (5)$$

The outgoing part, or the coefficient of e^{ikr}, is zero, or

$$\sum_{l=0}^{\infty} (2l+1) i^l A_l \exp\left[i\left(-\frac{(l+1)}{2}\pi - \delta_l\right)\right] P_l(\cos\theta) = \sum_{l=0}^{\infty} (2l+1) i^l \exp\left[i\left(-\frac{l+1}{2}\pi\right)\right] P_l(\cos\theta) , \quad (6)$$

so we get $A_l = e^{i\delta_l}$.

In so doing, we see that all the matrix elements are complex; $T_k^{(2)}$, we have

$$T_k^{(2)} = T_{0k0k}^{(2)} - T_{0kk0}^{(2)} - T_{0000}^{(2)} , \quad (7a)$$

$$T_{0000}^{(2)} = \frac{4\pi}{\Omega} \int_a^{R_{11}} dr\, r^2 v(r) \psi_{\text{ground}}(r) , \quad (7b)$$

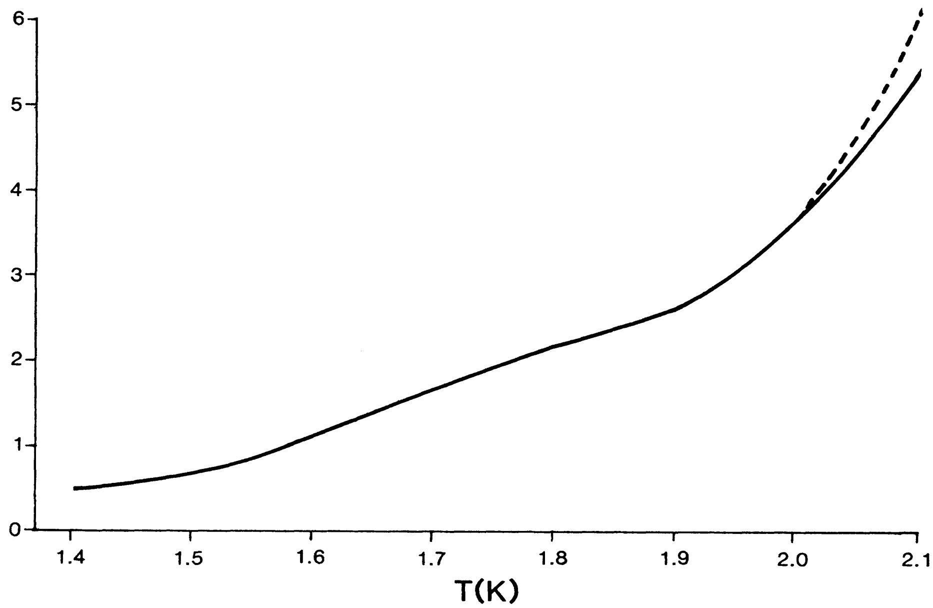

FIG. 1. S vs T, both experimental (——) and theoretical (---) results are shown.

and

$$T^{(2)}_{0k0k}+T^{(2)}_{0kk0}=\int \phi_{k/2}(\mathbf{r})v(r)\psi_{k/2}(\mathbf{r})r^2dr\,d\cos\theta d\varphi+\int \phi_{k/2}(\mathbf{r})v(r)\psi_{-k/2}(\mathbf{r})r^2dr\,d\cos\theta d\varphi$$

$$=\frac{8\pi}{\Omega}\sum_{\text{even}}\left\{e^{i\delta_l}\left[\frac{k}{2}\right](2l+1)\left[\cos\delta_l\left[\frac{k}{2}\right]\int_a^{R_{11}}dr\,r^2j_l^2\left[\frac{kr}{2}\right]v(r)\right.\right.$$

$$\left.\left.+\sin\delta_l\left[\frac{k}{2}\right]\int_a^{R_{11}}dr\,r^2j_l\left[\frac{kr}{2}\right]n_l\left[\frac{kr}{2}\right]v(r)\right]\right\}. \quad (7c)$$

For simplicity, we set $\psi_{\text{ground}}(r)=(r-a)/r$ with a the size of the hard core. It follows, therefore, that

$$T^{(2)}_{00k-k}=\frac{4\pi}{\sqrt{\Omega}}\int_a^{R_{11}}dr\,r^2v(r)\psi_k^{(0)}(r)\ , \quad (8)$$

and

$$T^{(2)}_{k-k00}=\frac{4\pi}{\Omega}\int_a^{R_{11}}dr\,r^2j_0(kr)v(r)\psi_{\text{ground}}(r)\ . \quad (9)$$

Here we will choose $\Omega=(4\pi R_{11}^3/3)$ and $R_{11}=4.1$ Å. We have made several calculations with different values of R_{11}, ranging from $R_{11}=3.5$ to $R_{11}=4.4$ Å. These seem to have a very small effect on the final answers. Ω is the true volume which each helium atom occupies. We notice that R_{11} is chosen to be 2.2 Å by Luban and Grobman.[5] This is much too small, for we have to choose the hard-core size to be 2.2 Å. The numerical values of the hard-core length, the potential $v(r)$, etc., are in accordance with the latest choices,[6,7] in which there is very little room for adjustment as the values are taken from experiment. However, this is a minor point. We see that the excitation spectrum $E_1(k,T)$ should be positive; we have, therefore, (otherwise we conform with Refs. 6 and 7),

$$E_1(k,T)=\left|\left[\frac{\hbar^2k^2}{2m}+Y+N_0T_k^{(2)}\right]^2-(Y+N_0T^{(2)}_{00k-k})(Y+N_0T^{(2)}_{k-k00})\right|^{1/2}, \quad (10a)$$

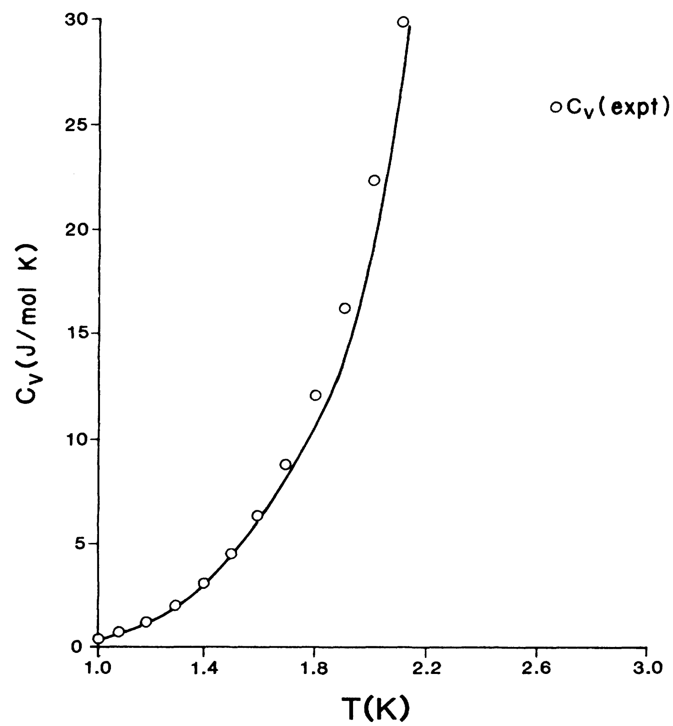

FIG. 2. C_v vs T. C_v experimental results are shown as open circles. C_v theoretical results are shown as a solid line.

TABLE I. S vs T.

T (K)	Entropy S (expt.) (J/mol K)	Entropy S (calc.) (J/mol K)
1.6	1.13	1.40
1.7	1.59	1.85
1.8	2.18	2.38
1.9	2.95	3.09
2.0	3.93	3.86
2.1	5.26	5.21

TABLE II. C_v vs T.

T (K)	C_v (expt.)	C_v (calc.)
1.6	6.42	7.86
1.7	8.82	9.56
1.8	12.1	11.5
1.9	16.3	14.0
2.0	22.4	18.5
2.1	30.0	29.4

and

$$Y=\frac{33\hbar^2\sin(ka)}{2kma^3} \quad (10b)$$

$|\cdots|$ represents the absolute value of the complex quantities inside. We take here the absolute value only for the sake of discussion. Namely, we leave the discussion of the roton lifetime to another paper. Here N_0 is temperature dependent and we take it as approximately

$$N_0=N\left[1-\left(\frac{T}{T_\lambda}\right)^{1.5}\right] . \quad (11)$$

Such a dependence on temperature is actually for ideal bosons with no hard-core interaction, as given, for example, in Huang's book.[8] Next we consider the quasiparticles. They have an energy given by Eq. (10). We see that their momentum vector k_1 is defined through

$$E_1(k,T)=\frac{\hbar^2k_1^2}{2m} . \quad (12)$$

We postulate here that the quasiparticles also interact with a hard core. Thus they are not simple particles anymore but, as interacting bosons, are subject to Hartree-Fock considerations. This gives not only the direct, but also the exchange part of the wave functions, which we will discuss in a later paper. We call this energy term $E(k,T)$, which is a modification of $E_1(k,T)$ by means of the Hartree-Fock method. For the quasiparticles, we use the temperature dependence[9] given by the experimental fit

$$N_0=N\left[1-\left(\frac{T}{T_\lambda}\right)^{5.6}\right] . \quad (13)$$

However, this relation can be derived and we will report the derivation of Eq. (13) later.

Since the energy depends on temperature, we cannot find, in the conventional way, the average of energy by differentiating the partition function with respect to temperature. Bendt, Cowan, and Yarnell[10] and Donnelly and Robert[11] give the entropy as

$$\frac{S}{N_A}=\frac{4\pi k}{\rho\hbar^3}\int_0^\infty\left[\frac{E(P,T)/k_BT}{e^{E(P,T)/k_BT}-1}-\ln(1-e^{-E(P,T)/k_BT})\right]p^2dp . \quad (14)$$

We get, therefore, with $\beta=(1/k_BT)$, $p=\hbar k$, and N_A Avogadro's number,

$$\frac{C_v}{N_A}=\frac{C_{v1}+C_{v2}}{N_A}=\frac{1}{N_A}T\left(\frac{\partial S}{\partial T}\right)_V=\frac{\beta k_B}{2\pi^2\rho}\left[\int_0^\infty\frac{\beta E^2e^{\beta E}}{(e^{\beta E}-1)^2}k^2dk+\int_0^\infty\frac{\partial E}{\partial\beta}\frac{\beta^2Ee^{\beta E}}{(e^{\beta E}-1)^2}k^2dk\right] . \quad (15)$$

In this expression, the second term C_{v2} will lead us to the understanding of why there is a further increase of C_v as $T\rightarrow T_\lambda$. We see that if we set $(\partial E/\partial\beta)=0$, Eq. (15) will reduce to the ordinary formula of $C_v\rightarrow T^3$.

In these expressions, we see that the calculated and the experimental entropy almost coincide. In Eq. (15), C_{v2} leads us to a further increase of C_v as $T\rightarrow T_\lambda$. This term is of considerable importance in obtaining agreement with the experimental data (see Figs. 1 and 2 and Tables I and II).

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*Present address: Physics Department, Ramkamhang University, Banggapi, Bangkok 10240, Thailand.

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