PHYSICAL REVIEW VOLUME 100, NUMBER 2 OCTOBER 15, 1955

λ Transition in Liquid Helium

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(Received March 24, 1955)

It is shown, by means of an expansion formula, that Feynman's partition function for liquid helium exhibits a second-order lambda transition. The validity of the expansion is discussed and it is shown that it is very likely to be valid for the case under consideration. A discussion is also given of some general properties of Feynman's partition function.

1. INTRODUCTION

In a recent publication[1] Feynman has proposed a comparatively simple approach to the problem of the phase transition in liquid helium. This approach consisted of constructing an alternative, exact, mathematical form for the partition function for liquid helium, and then using a series of intuitive physical arguments to derive from it a much simpler approximate partition function. We have discussed the derivation of this approximate partition function elsewhere[2] and we do not propose to enter into any further discussion of this aspect of Feynman's work in this paper. Unfortunately it is probably impossible, at least at the moment, to evaluate even this comparatively simple partition function. In his original paper[1] Feynman showed, using some rather crude approximations, that his partition function could exhibit a third-order transition under conditions of constant volume. It is a simple matter to show that it also exhibits a third-order transition under conditions of constant pressure. Recently several authors[2–5] have advanced opinions as to whether or not Feynman's form for the partition function can yield a second-order transition. This question is of some importance because if the partition function does exhibit such a transition then it will at least be in qualitative agreement with experiment.[6] Kikuchi has in fact shown, on the basis of a simple lattice model, that the partition function can exhibit a second order transition. He pointed out, however, that this result is not completely rigorous because of the unrealistic nature of the lattice model.

The purpose of this paper is to present what we believe is a fairly rigorous proof that Feynman's partition function does exhibit a second-order transition. Besides doing this we shall, however, discuss some general properties of Feynman's partition function.

Our proof of the existence of a second-order transition is based on an expansion formula for the partition function, Z. This function can be written as,[2]

$$Z=\frac{(\lambda')^{3N}}{N!}\int\cdots\int \exp[-\beta V'(\beta)] \times\rho_0(\mathbf{r}_1\cdots\mathbf{r}_N)d\mathbf{r}_1\cdots d\mathbf{r}_N, \quad (1.1)$$

where $(\lambda')^2=h^2/2\pi m'kT$, $\beta=1/kT$, m' is the effective mass introduced by Feynman and $V'(\beta)$ is the quasi interaction potential of the helium atoms.[2] The function $\rho_0(\mathbf{r}_1\cdots\mathbf{r}_N)$ is the probability density, in configuration space, for an ideal Bose Einstein gas of particles of mass m'. Finally the integral $\int\cdots\int\cdots d\mathbf{r}_1\cdots d\mathbf{r}_N$ indicates an integration over all the coordinates $\mathbf{r}_1\cdots\mathbf{r}_N$ of the helium atoms. Now Feynman has pointed out[1] that the essential property of the function $\exp(-\beta V')$ is that it must vanish whenever two or more helium atoms approach sufficiently close to one another. This simply means that configurations in which two or more atoms are very close together must be given zero weight in the partition function. Bearing this fact in mind we can construct a good approximation to the function $\exp(-\beta V')$ by assuming that $V'(\beta)$ is the potential energy for a system of N perfectly elastic spheres, the radii of which are independent of the temperature. This assumption does not imply any great loss of generality, for it preserves the essential property of the function and in addition any weak attractive or repulsive terms that may be present in $V'(\beta)$ can easily be taken into account by means of perturbation theory.[7] With this assumption we can write

$$\exp[-\beta V'(\beta)]=\prod_{i<j}^{N}[1+f(r_{ij})], \quad (1.2)$$

where $f(r_{ij})=f_{ij}$ is given by

$$\begin{aligned} f_{ij}&=-1; \quad r_{ij}\leqslant 2r_0\\ &=0; \quad r_{ij}>2r_0, \end{aligned} \quad (1.3)$$

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* Contribution No. 1283 from the Sterling Chemistry Laboratory.

[1] R. P. Feynman, Phys. Rev. **91**, 1291 (1953).

[2] G. V. Chester, Phys. Rev. **93**, 1412 (1954).

[3] D. ter Haar, Phys. Rev. **95**, 895 (1954).

[4] T. Matsubara, Busseiron Kenyku **72**, 78 (1954).

[5] R. Kikuchi, Phys. Rev. **96**, 563 (1954).

[6] W. H. Keesom, *Helium* (Elsevier Publishing Company, Inc., Amsterdam, 1942).

[7] In the second reference we showed how Feynman's partition function could be obtained from the full partition function by means of the semiclassical expansion in powers of h^2. However, if the interaction potential is singular over regions of configuration space, as is the case for perfectly elastic spheres, this method breaks down. This is simply because for this type of potential it is impossible to derive the usual expansion in powers of h^2. A very similar difficulty arises in the development of the perturbation expansion for the partition function. This has been discussed by the author in Phys. Rev. **93**, 606 (1954).

and r_0 is the radius of the elastic spheres. The expansion of the partition function which we shall construct is essentially an expansion in powers of Nr_0^3/V, where N/V is the density of the system. It should be pointed out that this expansion of Z is not identical with virial expansion and is therefore not necessarily divergent for a liquid phase. We shall return to this point later. In Sec. 2 we shall show how this expansion can be constructed and we shall calculate the first two terms of it explicitly.

In Sec. 3 we study the thermodynamic properties of the first two terms in this expansion and show that they lead to a second-order transition. Since this result is based on the first two terms in the expansion for Z we must try to decide whether or not it is true for the exact form for Z. We therefore conclude this section with a discussion of (a) the validity of the expansion formula itself and (b) the validity of breaking off the expansion after only two terms. The essential result that emerges from this discussion is that the results we have derived by our approximate method are very likely to be true for the exact form for Z. We have not, however, been able to construct a completely rigorous argument to show this.

Finally in Sec. 4 we discuss some general properties of Feynman's partition function.

2. THE EXPANSION FORMULA

We first construct an explicit expression for $\rho_0(\mathbf{r}_1\cdots\mathbf{r}_N)$. This function is the unnormalized probability density, in configuration space, for a system of N noninteracting particles of mass m'. If the eigenvalues of Schrödinger's equation for such a system are E_l and if ϕ_l are the corresponding, correctly symmetrized, wave functions then

$$[(\lambda')^{3N}/N!]\rho_0(\mathbf{r}_1\cdots\mathbf{r}_N)=\textstyle\sum_l\phi_l^*\phi_l\exp[-\beta E_l]. \qquad (2.1)$$

Substituting this expression in Eq. (1.1), we get,

$$Z=\sum_l\left[\int\cdots\int\phi_l^*\exp(-\beta V')\phi_l d\mathbf{r}_1\cdots d\mathbf{r}_N\right]\times\exp(-\beta E_l), \qquad (2.1)$$

and if we define R_{ll} by the equation

$$R_{ll}=\int\cdots\int\phi_l^*\exp[-\beta V']\phi_l d\mathbf{r}_1\cdots d\mathbf{r}_N, \qquad (2.2)$$

then

$$Z=\textstyle\sum_l R_{ll}\exp[-\beta E_l]. \qquad (2.4)$$

This last equation can be rewritten in the form

$$Z=Z_0\langle R_{ll}\rangle^0, \qquad (2.5)$$

where

$$Z_0=\textstyle\sum_l\exp(-\beta E_l), \qquad (2.6)$$

and

$$\langle R_{ll}\rangle^0=\textstyle\sum_l R_{ll}\exp(-\beta E_l)/\sum_l\exp(-\beta E_l). \qquad (2.7)$$

It follows at once that the free energy F can be written as

$$F=F_0+F_1, \qquad (2.8)$$

where

$$F_0=-kT\log Z_0;\quad F_1=-kT\log\langle R_{ll}\rangle^0. \qquad (2.9)$$

So far we have made no approximations. We now wish to develop an expansion formula for F_1. To do this we substitute into Eq. (2.3) the expression given by Eq. (1.2) for $\exp(-\beta V')$. Thus,

$$R_{ll}=\int\cdots\int\phi_l^*\phi_l\prod_{i<j}(1+f_{ij})d\mathbf{r}_1\cdots d\mathbf{r}_N. \qquad (2.10)$$

The integral on the right hand side of Eq. (2.10) is very similar to the configuration integral that arises in the classical theory of compressed gases.[8] In fact if we put $\phi_l^*\phi_l\equiv 1$, then the integrals become identical. This suggests that we can probably obtain an expansion for F_1 by using the same techniques[8] that are used to develop the cluster expansion of the classical configuration integral. This surmise proves to be correct and it will clarify our work if we briefly recall the main steps in the calculation of the first two terms in the classical cluster expansion.

In the classical case we have to consider the integral

$$K=\int\cdots\int\prod_{i<j}(1+f_{ij})d\mathbf{r}_1\cdots d\mathbf{r}_N. \qquad (2.11)$$

The first step is to expand the product $\prod_{i<j}(1+f_{ij})$ as a polynomial, the terms of which are sums of products of the f_{ij}. Thus,

$$\prod_{i<j}(1+f_{ij})=1+\sum_{i<j}f_{ij}+\sum_{i_1<j_1}\sum_{i_2<j_2}f_{i_1j_1}f_{i_2j_2}\cdots. \qquad (2.12)$$

We next integrate this expansion over all the coordinates. The first term is trivial and leads at once to a term V^N. To obtain the first-order correction to this term we simply have to select from each term in the polynomial just those terms in which there are no f_{ij}'s with common suffices. For example in the first sum, $\sum_{i<j}f_{ij}$, as there are no terms with more than one f_{ij} we keep all the terms. In the second sum, however, we select terms like $f_{ij}f_{kl}$ but reject terms like $f_{ij}f_{jk}$. In the rth sum in the polynomial each term consists of r f_{ij}'s multiplied together, and as we only retain terms with no common suffices this means that we have $2r$ different coordinates appearing in the f_{ij}, and $N-2r$ that do not appear. Therefore when we integrate over all the coordinates, $N-2r$ of these integrations can be carried out at once to yield a factor V^{N-2r}. The remaining $2r$ integrations can also be easily performed—simply because there are no common suffixes in the product of the f_{ij}'s—and yield a factor z^r, where z^r is

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[8] R. H. Fowler, *Statistical Mechanics* (Cambridge University Press, Cambridge, 1936), Chap. 8.

given by

$$z=\int_{\rho} f(\boldsymbol{\varrho})d\boldsymbol{\varrho}, \qquad (3.13)$$

and $\boldsymbol{\varrho}$ is equal to $\mathbf{r}_i-\mathbf{r}_j$. Consequently from any one term in the rth sum we get a contribution $V^{N-r}z^r$. To get the complete contribution to K from the sum we multiply this typical contribution by the number of terms we retain. This number is just the number of ways of picking r different pairs of suffixes from a total of N suffixes. If this number is denoted by $P(r,N)$, then the total contribution to K from the rth sum is $P(r,N)V^{N-r}z^r$. We now have to sum this expression over all values of r from 0 to $N/2$ to obtain, to our degree of approximation, the complete expression for K, namely,

$$K=\sum_{r=0}^{N/2} P(r,N)V^{N-r}z^r=V^N\sum_{r=0}^{N/2} P(r,N)N^{-r}2^rx^r, \qquad (2.14)$$

where

$$x=\frac{N}{2V}\int_{\boldsymbol{\varrho}} f(\boldsymbol{\varrho})d\boldsymbol{\varrho}, \qquad (2.15)$$

and depends on N and V only through the density N/V. It is now a fairly simple matter to show[8] that for sufficiently large N the sum in Eq. (2.14) is asymptotically equal to $(1+x)^N$, to first order in x. Therefore $\log K$ is is given by,

$$\log K=N\log V+N\log(1+x)\doteqdot N\log V+Nx. \qquad (2.16)$$

This completes the evaluation of $\log K$ to the desired degree of approximation. We shall now show that a very similar cluster expansion can be obtained for $\log\langle R_{ll}\rangle^0$.

The wave functions that appear in the integral, Eq. (2.10), for R_{ll} are the correctly symmetrized wave functions for N noninteracting point particles of mass m'. They can be written as,

$$\phi_l(\mathbf{r}_1\cdots\mathbf{r}_N)=A_l\sum_P\exp[2\pi iP\sum_{j=1}^N\mathbf{k}_j\cdot\mathbf{r}_j], \qquad (2.17)$$

where A_l is a normalization constant, P is a permutation operator acting on the N suffixes of the wave vectors $\mathbf{k}_j$, $\sum_P$ indicates a summation over all distinct permutations P and $\sum_j$ is a sum over all N indices j. From this last equation we have that,

$$\phi_l^*\phi_l=A_lA_l^*\sum_P\sum_{P'}$$
$$\times\exp[2\pi i(P\sum_{j=1}^N\mathbf{k}_j\cdot\mathbf{r}_j-P'\sum_{j'=1}^N\mathbf{k}_{j'}\cdot\mathbf{r}_{j'})]. \qquad (2.18)$$

Substituting this expression into Eq. (2.10) we have

$$R_{ll}=A_lA_l^*\sum_P\sum_{P'}R_{ll}(P,P'), \qquad (2.19)$$

where

$$R_{ll}(P,P')$$
$$=\int\cdots\int\exp[2\pi i(P\sum_{j=1}^N k_j\cdot r_j-P'\sum_{j'=1}^N k_{j'}\cdot r_{j'})]$$
$$\times\sum_{i<j}(1+f_{ij})d\mathbf{r}_1\cdots d\mathbf{r}_N. \qquad (2.20)$$

We now expand the product $\prod_{i<j}(1+f_{ij})$ in the same way as before and we again select only those terms from the rth sum in the expansion that have no common suffices. This procedure yields the following series for $R_{ll}(P,P')$,

$$R_{ll}(P,P')=\sum_{r=0}^{N/2}P(r,N)N^{-r}J_{l,r}(P,P'), \qquad (2.21)$$

where

$$J_{l,r}(P,P')=\int\cdots\int f_{ij}f_{kl}\cdots f_{\mu\sigma}$$
$$\times\exp[2\pi i(P\sum_{j=1}^N\mathbf{k}_j\cdot\mathbf{r}_j-P'\sum_{j'=1}^N k_{j'}\cdot r_{j'})]. \qquad (2.22)$$

We now substitute this series for $R_{ll}(P,P')$ into Eq. (2.19) and get

$$R_{ll}=A_lA_l^*\sum_P\sum_{P'}\sum_{r=0}^{N/2}P(r,N)N^{-r}J_{l,r}(P,P'). \qquad (2.23)$$

If we invert the order of summation, this leads to

$$R_{ll}=\sum_{r=0}^{N/2}P(r,N)N^{-r}H_{l,r}, \qquad (2.24)$$

where $H_{l,r}$ is given by

$$H_{l,r}=A_lA_l^*\sum_P\sum_{P'}J_{l,r}(P,P'). \qquad (2.25)$$

The evaluation of the integrals in Eq. (2.22) and the summation in Eq. (2.25) involve elementary but lengthy operations. These are carried out in Appendix A where it is shown that $H_{l,r}$ is given by

$$H_{l,r}=(I_l)^r=(N/V)^r\left[\int_{\boldsymbol{\varrho}} f(\boldsymbol{\varrho})g_l(\boldsymbol{\varrho})d\boldsymbol{\varrho}\right]^r, \qquad (2.26)$$

where

$$g_l(\boldsymbol{\varrho})=(1/N^2)\sum_{\mathbf{k}\neq\mathbf{k}'}\sum n_{\mathbf{k}}n_{\mathbf{k}'}\exp[2\pi i\boldsymbol{\varrho}\cdot(\mathbf{k}-\mathbf{k}')]+1, \qquad (2.27)$$

and the symbols $n_{\mathbf{k}}$ that appears in this last equation are the set of integers that define the state l; they give the number of wave vectors in the wave function ϕ_l that are equal to $\mathbf{k}$, and satisfy the relation $\sum_{\mathbf{k}}n_{\mathbf{k}}=N$. We see that the only difference between the integral for I_l and the corresponding classical integral for x is the extra factor $g_l(\boldsymbol{\varrho})$ in the integrand. This function, considered as a function of N and V, is of order unity.

We have at once from Eq. (2.24) that

$$\langle R_{ll}\rangle^0=\sum_{r=0}^{N/2} P(r,N)N^{-r}\langle(I_l)^r\rangle^0. \tag{2.28}$$

It is shown in Appendix B that to our degree of approximation $\langle(I_l)^r\rangle^0$ can be replaced by $(\langle I_l\rangle^0)^r$; we then have

$$\langle R_{ll}\rangle^0=\sum_{r=0}^{N/2} P(r,N)N^{-r}(\langle I_l\rangle^0)^r, \tag{2.29}$$

and for large N this gives,

$$\langle R_{ll}\rangle^0\simeq(1+\tfrac{1}{2}\langle I\rangle^0)^N. \tag{2.30}$$

From Eq. (2.9), we have

$$F_1=-kT\log\langle R_{ll}\rangle^0\simeq-\frac{NkT}{2}\langle I_l\rangle^0, \tag{2.31}$$

where

$$\langle I_l\rangle^0=(N/V)\int_{\boldsymbol{\varrho}} f(\boldsymbol{\varrho})\langle g_l(\boldsymbol{\varrho})\rangle^0 d\boldsymbol{\varrho}, \tag{2.32}$$

and

$$\langle g_l(\rho)\rangle^0=(1/N^2)\sum_{\mathbf{k}\neq\mathbf{k}'}\sum \bar{n}_{\mathbf{k}}\bar{n}_{\mathbf{k}'}\exp[2\pi i\rho\cdot(\mathbf{k}-\mathbf{k}')]+1. \tag{2.33}$$

In this last equation the $\bar{n}_{\mathbf{k}}$ are the mean values of the integers $n_{\mathbf{k}}$ that appeared in Eq. (2.26). Since $f(\boldsymbol{\varrho})$ differs from zero only if $|\boldsymbol{\varrho}|\leqslant 2r_0$, we see that $\langle I_l\rangle^0 \sim Nr_0^3/V$, and is therefore of exactly the same order of magnitude as the first term in the classical cluster expansion. It is easily shown that if we include in our calculations more complicated products of f_{ij}'s then we get terms in the expansion of F_1, that depend on higher powers of Nr_0^3/V. We shall not, however, calculate any of these terms as they are unnecessary for our purpose.

3. NATURE OF THE TRANSITION

If we combine Eq. (2.32) and Eq. (2.31), invert the order of integration and summation and then substitute the result in Eq. (2.30) we get,

$$F_1=\tfrac{1}{2}\sum_{\mathbf{k}\neq\mathbf{k}'}\sum \bar{n}_{\mathbf{k}}\bar{n}_{\mathbf{k}'}L_{\mathbf{k},\mathbf{k}'}+\tfrac{1}{2}N^2L_0, \tag{3.1}$$

where

$$L_{\mathbf{k},\mathbf{k}'}=\frac{1}{V}\int_{\boldsymbol{\varrho}}\exp[2\pi i\boldsymbol{\varrho}\cdot(\mathbf{k}-\mathbf{k}')][-kTf(\boldsymbol{\varrho})]d\boldsymbol{\varrho}, \tag{3.2}$$

and

$$L_0=\frac{1}{V}\int_{\boldsymbol{\varrho}}[-kTf(\boldsymbol{\varrho})]d\boldsymbol{\varrho}. \tag{3.3}$$

Now the $\bar{n}_k$ that occur in Eq. (3.1) are, as we have pointed out in the previous section, the average values of the integers $n_{\mathbf{k}}$ that define the state l. Since these averages were calculated with weights $\exp(-\beta E_l)/\sum\exp(-\beta E_l)$, the $\bar{n}_k$ must be identical with the average occupation numbers of the single particle energy levels of an ideal Bose-Einstein gas. We summarize the properties[9] of these occupation numbers,

$$\bar{n}_{\mathbf{k}}=[\exp(\mu k^2+\alpha)-1]^{-1},\quad \text{all }\mathbf{k};\quad T>T_\lambda, \tag{3.4}$$

$$\bar{n}_{\mathbf{k}}=[\exp(\mu k^2)-1]^{-1},\quad \mathbf{k}>0;\quad T\leqslant T_\lambda, \tag{3.5}$$

and

$$\bar{n}_0=N-\sum_{\mathbf{k}\neq 0}\bar{n}_{\mathbf{k}}.\quad T\leqslant T_\lambda$$

Here $\mu=\hbar^2/2m'kT$, the transition temperature T_λ is given by

$$T_\lambda=(h^2/2m'k\pi)[N/V\zeta(\tfrac{3}{2})]^{\frac{2}{3}}, \tag{3.6}$$

and $\zeta(\frac{3}{2})$ is the Riemann zerta function of order $\frac{3}{2}$. The statistical parameter α is given as a function of T and N/V by the equation $\sum_{\mathbf{k}}\bar{n}_{\mathbf{k}}(\alpha;\,T,V)=N$, for $T>T_\lambda$. For $T\leqslant T_\lambda$ α is identically zero.[9] It follows from this last equation that α and its first order derivatives with respect to T and V are continuous at T_λ but that all the higher order derivatives are discontinuous at this temperature. Equations (3.4) and (3.5) define the $\bar{n}_{\mathbf{k}}$ as functions of T, V, and α, and we shall henceforth consider F_1 to be given as a function of these variables. The term F_0 in Eq. (2.7) is very easily evaluated as it is the free energy of an ideal Bose-Einstein gas composed of particles of mass m'. It is given explicitly by the equations

$$F_0=-NkT\alpha+kT\sum_{\mathbf{k}}\log[1-\exp(-\mu k^2-\alpha)];\quad T>T_\lambda, \tag{3.7}$$

and

$$F_0=kT\sum_{\mathbf{k}}\log[1-\exp(-\mu k^2)];\quad T\leqslant T_\lambda. \tag{3.8}$$

Here all the symbols have exactly the same meaning as before. If we regard Eq. (3.7) as defining F_0 as an explicit function of T, V, and α, then it is easily seen that $[\partial F_0/\partial\alpha]_{T,V}\equiv 0$; this last relation is in fact equivalent to the equation $\sum_{\mathbf{k}}\bar{n}_k(\alpha,T,V)=N$, which the $\bar{n}_{\mathbf{k}}$ must satisfy.

We can now use exactly the same arguments that we used in a previous publication[10] to show that, while F_0 exhibits a third-order transition at T_λ, F_1, exhibits a second order transition at this temperature. We first notice that because $[\partial F_0/\partial\alpha]_{T,V}\equiv 0$, the rth derivatives of F_0 with respect to T and V only depend on the $(r-1)$th and lower order derivatives of α. Since only the second and higher order derivatives of α are discontinuous at T_λ it follows that only the third and higher order derivatives of F_0 will be discontinuous at this temperature. This result is of course to be expected because F_0 is merely the free energy of an ideal Bose-Einstein gas, and such a system exhibits a third order transition under conditions of constant volume. It is easily seen from Eq. (3.1) that $[\partial F_1/\partial\alpha]_{T,V}\neq 0$. Therefore the rth derivatives of F_1 will depend on the rth derivatives of α. This in turn implies that the second-order derivatives of F_1 will be discontinuous at

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[9] A. R. Fraser, Phil. Mag. **42**, 156, 165 (1951).

[10] G. V. Chester, Phys. Rev. **94**, 246 (1954).

T_λ and that F_1 will exhibit a second-order transition under conditions of constant volume. To show that it exhibits a second-order transition under conditions of constant pressure we merely have to show that $(\partial p/\partial V)_T < 0$, for $T \leqslant T_\lambda$. This inequality also determines whether the system is stable for $T \leqslant T_\lambda$. Because $(\partial p/\partial V)_T \equiv 0$, for $T \leqslant T_\lambda$, in the London theory this theory leads to a first-order transition under conditions of constant pressure. It is easily shown[11] that the first term in Eq. (3.1) is linear in V, for $\leqslant T_\lambda$; therefore $(\partial p/\partial V)_T$ is given by[12]

$$(\partial p/\partial V)_T = (-N/V^2) \int_{\varrho} [-kTf(\varrho)] d\varrho. \qquad (3.9)$$

Consequently $(\partial p/\partial V)_T < 0$ as long as $\int_{\varrho} [-kTf(\varrho)] d\varrho > 0$. From the definition of $f(\varrho)$, Eq. (1.3), we have at once the integral $= 4\pi MkTr_0^3/3V^2$, and is therefore positive. We have therefore shown that to our degree of approximation the partition function proposed by Feynman exhibits a second-order transition both under conditions of constant pressure and under conditions of constant volume. For the sake of completeness we quote the formula for the discontinuity in the specific heat at constant volume. If $\Delta C_V = C_V(T_\lambda + 0) - C_V(T_\lambda - 0)$, then

$$\Delta C_V = 4\pi N \frac{N}{V} \frac{T_\lambda^2}{\zeta^2} \left(\frac{\partial^2 \alpha}{\partial T^2} \right)_{T=T_\lambda} \int_0^\infty [-kTf(\varrho) \times S(\rho) T(\varrho)] \rho^2 d\rho, \qquad (3.10)$$

where

$$S(\rho) = \sum_{n=1}^{\infty} \exp(-a\rho^2/n)/n^{\frac{3}{2}},$$

$$T(\rho) = \sum_{n=1}^{\infty} [1 - \exp(-a\rho^2/n)]/n^{\frac{1}{2}}$$

and $a = \pi/\lambda'$.

It is interesting to examine, in a more physical manner, the reason why the second term in the expansion changed the transition from one of the third order to one of the second order. In the first term in the series the transition arises because of the existence of very large cyclical configurations, or polygons, in the integrand of the partition function. This fact has been pointed out by Feynmann.[1] Now it is well known that in the type of cluster expansion we have used the second term in the expansion always introduces correlation between the atoms. In particular this means that we have introduced correlation between the polygons in the integrand of the partition function. It is just the introduction of these correlations that changes the order of the transition. As long as the polygons are uncorrelated we shall have a third-order transition, but as soon as we introduce correlation between them the transition changes to a second-order one.

Finally we note that if T_λ, as given by Eq. (3.6), is to agree with experiment we must have then $m' \sim \frac{3}{2} m$ at the λ temperature. We also note that $\partial T_\lambda / \partial \rho$ will only have the correct sign if m' varies with ρ faster than $\rho^{\frac{2}{3}}$. While both these requirements seem to be reasonable on physical grounds we cannot see any rigorous method of showing that they are satisfied.

We now turn to a discussion of the validity of these results, the point at issue being whether they are true for the exact form of Feynman's partition function or whether they are spurious and result from the approximations that we have made. The two essential steps in our method are (a) the development of the expansion formula itself and (b) the approximation of breaking off this expansion after only two terms. We shall discuss these points in turn.

The use of an expansion formula for F_1 could only lead to incorrect results if it were divergent. To develop the complete series for F_1 along the lines we have suggested would be an extremely tedious task and a rigorous proof, or disproof, of the convergence of the series would be almost impossible. It would therefore seem to be worth while to present a much simpler physical argument that suggests that the series for F_1 is convergent at the temperatures and densities we are interested in. Our argument is based on the fact that if we set $\phi_l \phi_l^* \neq 1$ in the integral for R_{ll} then this integral becomes identical with the classical configuration integral for N perfectly elastic spheres; our expansion formula is then identical with the classical virial expansion. Now since the coefficients of this expansion are independent of the temperature its radius of convergence will also be independent of the temperature. It seems reasonable on physical grounds to suppose that this series will be convergent for sufficiently low densities, and, since the density of liquid helium is only about one half the density of a "normal" fluid, it is reasonable to suppose that the series will be convergent at liquid helium densities. Now the only difference between the coefficients in the classical expansion and those in the expansion we have proposed is that in the integrals that define the coefficients we have an extra factor $\phi_l \phi_l^*$. This factor is always positive, less than unity and, in the region we are interested in, is a slowly varying function of the coordinates. Bearing these facts in mind it seems possible that the introduction of this extra factor into the integrals will in fact leave the radius of convergence of the series almost unaltered. On the basis of this very incomplete and unrigorous argument it is plausible that the expansion we have proposed for F_1 is convergent at the temperatures and densities we are interested in.

If this conclusion is correct then we only have to show that the results we have obtained on the basis of

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[11] G. V. Chester, Phys. Rev. **100**, 446 (1955).

[12] This formula is correct as long as the dependence of m' on V is ignored. If this dependence is taken into account then the expression for $(\partial p/\partial V)_T$ becomes more complicated. It is easily seen, however, that $(\partial p/\partial V)_T \neq 0$ and that in consequence the transition remains a second order one.

the first two terms in the series will not be altered by taking into account the behavior of any of the higher terms in it. We in fact showed that the second order derivatives of the second term in the expansion of F_1 were discontinuous at a temperature T_λ given by Eq. (3.6). If this result is spurious then the derivatives of the higher order terms in the series must also be discontinuous at this temperature. Moreover these discontinuities must be just sufficient to cancel out those that we have found. It is very easily seen that our expansion of F_1 is essentially an expansion in powers of Nr_0^3/V. Consequently while the discontinuities in the various terms may exactly cancel for one particular value of Nr_0^3/V it would seem to be impossible that they should do so in general. We can therefore conclude that the discontinuities we have found are in fact genuine. On the other hand it should be pointed out that there is nothing to prevent the first-order derivatives of any of the higher order terms in the series exhibiting discontinuities; this type of behavior would lead to a first order transition. We can therefore conclude that while it seems fairly certain that Feynman's partition function exhibits a second-order λ transition we cannot rule out the possibility that it exhibits a first-order λ transition.

4. SOME GENERAL CONSIDERATIONS

First we wish to draw attention to an important theoretical point that must be considered whenever we construct a theory of liquid helium. A helium atom consists of two electrons that are tightly bound to a nucleus, and we normally treat this composite system as an individual particle. Moreover since the total spin of this system, when it is in the ground state, is zero we must apply Bose-Einstein statistics to any assembly of them. However, this procedure is only correct as long as the two electrons can be considered as being so tightly bound to the nucleus that the whole system behaves as a rigid particle. This is of course well known.[13] Now if in any statistical treatment of a system composed of helium atoms we allow configurations to occur in which two or more atoms come so close together that their charge clouds overlap, then we cannot apply Bose-Einstein statistics to the atoms in these configurations. In other words, in configurations of this type we must not symmetrize the total wave function with respect to the coordinates of the atoms but we must rather antisymmetrize it with respect to the coordinates of the individual electrons and nucleons that go to make up the atoms. For this reason, it is not possible to regard London's ideal gas theory as an accurate treatment of a noninteracting system of helium atoms, although it is of course an accurate treatment of a system of noninteracting Bose-Einstein particles. For example, it is clear from the Pauli exclusion principle that the probability of finding two collections of electrons and nuclei in the same region of configuration space will be very small. London's treatment, on the other hand, indicates that there is a very high probability of this happening.

Let us now examine Feynman's partition function in the light of these remarks. It follows from Eq. (1.1) that Feynman gives each configuration a statistical weight $\rho_0 \exp(-\beta V')$. Therefore as long as the function $\exp(-\beta V')$ vanishes whenever two or more helium atoms approach very close together this configuration density will be perfectly satisfactory. To be more precise this means that the function $\exp(-\beta V')$ must vanish, or at least become very small, whenever any of the $N(N-1)/2$ conditions $r_{ij} \leqslant 2r_0$ (where r_0 is the radius of the charge cloud of a helium atom) are satisfied. However, we have pointed out that this is an essential property of the function $\exp(-\beta V')$. We can therefore conclude that the configurational density that Feynman has proposed fulfills the requirements we have discussed above. It is easily shown that our approximate method of dealing with the partition function is also satisfactory in this respect.

Finally we wish to discuss whether Feynman's partition function can exhibit a liquid-gas transition. This question is important because the λ transition only takes place in the liquid phase of helium. Consequently any really satisfactory theory of liquid helium must (a) show that helium exhibits a liquid-gas transition and (b) show that this transition takes place at a temperature above the theoretical λ transition. It appears likely that Feynman's treatment can fulfill at least the first of these requirements. This conclusion rests on the following considerations. The function $\rho(\mathbf{r}_1 \cdots \mathbf{r}_N)$, that occurs in the integrand of the partition function, is of the form $1+f(\mathbf{r}_1 \cdots \mathbf{r}_N)$. Here $f(\mathbf{r}_1 \cdots \mathbf{r}_N)$ is a sum of terms each of which contains at least one factor of the type $\exp[-(8\pi r_0^2/\lambda^2)x_{ij}^2]$, where $x_{ij}=r_{ij}/2r_0$ and $\lambda = h^2/2\pi mkT$. Since the other factor in the integrand vanishes whenever $x_{ij} \leqslant 1$ the smallest value that the argument of the exponential can have is $8\pi r_0^2/\lambda^2$. This in turn implies that the function $f(\mathbf{r}_1 \cdots \mathbf{r}_N)$ falls very rapidly to zero, as any pair of relative coordinates increases, as long as $T \gg 2$°K. Thus for temperatures above about 6°K the factor ρ_0 may be replaced by unity. In this region of temperature therefore the partition function reduces to exactly the same form as the partition function for a classical fluid except that the actual potential V is replaced by the quasi potential $V'(\beta)$. Now as long as $V'(\beta)$ contains a weak attractive part this partition function will exhibit a gas-liquid transition. Unfortunately we cannot estimate the temperature at which this will occur unless we know something of the form of $V'(\beta)$, and this means that we cannot be sure that even if a transition takes place it will occur at a temperature above the λ point. However, it is worth noting that if V' is set equal to the true interaction potential, V, then it is almost certain that the partition function will exhibit a gas-liquid transition at about 13°K. For we know from the law of

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[13] R. H. Fowler, reference 8, Chap. 2.

corresponding states that if helium were a "classical" liquid it would liquify at about this temperature. Now at 13°K the factors $\exp(-kr^2)$ that occur in the function $f(\mathbf{r}_1\cdots\mathbf{r}_N)$ are never greater than 10^{-3}, in the region of configuration space of interest, and hence we can certainly set $f\equiv 0$ and $\rho_0\equiv 1$. The partition function then becomes identical with that for a classical fluid, with an interaction potential V, and will therefore exhibit a gas-liquid transition at about 13°K. This shows that this approximation to the partition function does not take into account the high zero-point energy of liquid helium. To introduce the zero-point energy in this approximation we have to assume that the quasi potential, V', is much weaker than the actual potential V. On the basis of this assumption it is probably fairly simple to construct a realistic "model" of liquid helium near the λ point; it remains to be shown how such a "model" can be derived from first principles. As we have already mentioned, the weak attractive part of the potential, that is necessary for a gas-liquid condensation, can easily be taken account of near the λ temperature by means of perturbation theory.

The author wishes to thank the United States Government for the award of an F. O. A. research fellowship.

APPENDIX A

In this Appendix, we shall outline the main steps in the evaluation of the integral for $J_{l,r}(P,P')$, Eq. (2.22), and the sum for $H_{l,r}$, Eq. (2.25).

We first consider the integral for $J_{l,s}(P,P')$,

$$J_{l,s}(P,P')=\int\cdots\int f(1,2)f(3,4)\cdots f(2s-1,\,2s)\times\exp\Big[2\pi i\Big(P\sum_{j=1}^{N}\mathbf{k}_j\cdot\mathbf{r}_j-P'\sum_{j'=1}^{N}\mathbf{k}_{j'}\cdot\mathbf{r}_{j'}\Big)\Big]d\mathbf{r}_1\cdots d\mathbf{r}_N,\quad\text{(A.1)}$$

where $f(i,k)$ stands for $f(r_{ik})$. Let us suppose that P and P' are a pair of permutations that permute the indices (j) on the wave vectors k in the following way,

$$P(1\cdots N)=(\alpha_1\cdots\alpha_N),\quad\text{(A.2)}$$

and

$$P'(1\cdots N)=(\alpha_1'\cdots\alpha_N').\quad\text{(A.3)}$$

These two equations are to be interpreted as meaning that when P operates on the indices $1\cdots N$ it sends them into a permutation $\alpha_1\cdots\alpha_N$ and similarly for P'. There are $(N-2r)$ coordinates that do not appear in the functions $f(i,k)$. We can therefore integrate over these coordinates at once. Because of the orthogonality conditions on the single particle wave functions, $\exp[2\pi i\mathbf{k}\cdot\mathbf{r}]$, the integration over the ith of these coordinates yields a factor $V\delta(\alpha_i,\alpha_i')$, where $\delta(\alpha,\beta)$ is zero if $\alpha\neq\beta$ and unity if $\alpha=\beta$. Consequently, $J_{l,s}(P,P')$ will vanish unless $\alpha_i=\alpha_i'$, for all $i>2s$. When these conditions are fulfilled the integral reduces to,

$$J_{l,s}(P,P')=V^{N-2s}\int\cdots\int f(1,2)f(3,4)\cdots f(2s-1,\,2s)\times\exp\Big[2\pi i\Big(P\sum_{j=1}^{2s}\mathbf{k}_j\cdot\mathbf{r}_j-P'\sum_{j'=1}^{2s}k_{j'}\cdot r_{j'}\Big)\Big]d\mathbf{r}_1\cdots d\mathbf{r}_{2s}.\quad\text{(A.4)}$$

Next we introduce center of mass and relative coordinates for each pair of coordinates that appear together in a function $f(i,\,i+1)$. Thus,

$$\boldsymbol{\varrho}_i=(\mathbf{r}_i-\mathbf{r}_{i+1})/2;\quad \mathbf{R}_i=(\mathbf{r}_i+\mathbf{r}_{i+1})/2;\quad (i=1,\,3,\,\cdots,\,2s-1).\quad\text{(A.5)}$$

Solving these equations we get,

$$\mathbf{r}_i=\mathbf{R}_i+\boldsymbol{\varrho}_i;\quad \mathbf{r}_{i+1}=\mathbf{R}_i-\boldsymbol{\varrho}_1;\quad (i=1,\,3\cdots,2s-1),\quad\text{(A.6)}$$

and the integral now becomes

$$J_{l,s}(P,P')=V^{N-2s}\int\cdots\int f(\boldsymbol{\varrho}_1)\cdots f(\boldsymbol{\varrho}_{2s-1})\times\exp\Big\{2\pi i\sum_{i=1,3\cdots}^{2s-1}\mathbf{R}_i[P(\mathbf{k}_i+\mathbf{k}_{i+1})-P'(\mathbf{k}_i+\mathbf{k}_{i+1})]\Big\}\times\exp\Big\{2\pi i\sum_{i=1,3\cdots}^{2s-1}\boldsymbol{\varrho}_i[P(\mathbf{k}_i-\mathbf{k}_{i+1})-P'(\mathbf{k}_i-\mathbf{k}_{i+1})]\Big\}\times d\boldsymbol{\varrho}_1\cdots d\boldsymbol{\varrho}_{2s-1}d\mathbf{R}_1\cdots d\mathbf{R}_{2s-1}.\quad\text{(A.7)}$$

If we perform the integrations over the center-of-mass coordinates $\mathbf{R}_j$, we find that $J_{l,s}(P,P')$ vanishes unless the s conditions,

$$\mathbf{k}(\alpha_i)+\mathbf{k}(\alpha_{i+1})=\mathbf{k}(\alpha_i')+\mathbf{k}(\alpha_{i+1}'),\quad (i=1,\,3\cdots,\,2s-1).\quad\text{(A.8)}$$

are satisfied. Here $\mathbf{k}(\mu)$ stands for $\mathbf{k}_\mu$. These conditions can be fulfilled in two ways: (a) by choosing P and P' so that they are satisfied identically for all values of the wave vectors $\mathbf{k}$ or (b) by regarding them as conditions to be imposed on the wave vectors. We ignore this second possibility for the moment; we shall show later that if one or more of the s conditions are imposed on the wave vectors then the contribution to $H_{l,s}$ is negligible. Let us return to the first possibility. For any given P the conditions given by Eq. (A.8) can only be satisfied if P' is such that either $\alpha_i'=\alpha_i$ and $\alpha_{i+1}'=\alpha_{i+1}$, or $\alpha_i'=\alpha_{i+1}$ and $\alpha_{i+1}'=\alpha_i$, for all $i=1,\,3\cdots,\,2s-1$. Let us suppose therefore that P' is a permutation such that $\alpha_i=\alpha_{i+1}'$ and $\alpha_{i+1}=\alpha_i'$, for $1\leqslant i\leqslant p$; while $\alpha_{i+1}'=\alpha_{i+1}$ and $\alpha_i'=\alpha_i$, for $p<i\leqslant 2s-1$. Then the integral for

$J_{l,s}(P,P')$ becomes

$$J_{l,s}(P,P')=J_{l,s}(P,p)$$

$$=V^{N-s}\left[\int_{\varrho} f(\varrho)d\varrho\right]^{s-p}\int\cdots\int f(\rho_1)\cdots$$

$$\times f(\varrho_p)\exp\left[2\pi i\sum_{i=1}^{p}\varrho_i(\mathbf{k}_i-\mathbf{k}_{i+1})\right]d\varrho_1\cdots d\varrho_p,$$

where we have relabeled the wave vectors for convenience, $k_i=k(\alpha_i)$, and we have replaced P' in $J_{l,s}(P,P')$ by p to indicate that P' is identical with P except that p of the N indices on the k's are permuted in pairs, namely so that $\alpha_i'=\alpha_{i+1}$ and $\alpha_{i+1}'=\alpha_i$, for $1\leqslant i\leqslant p$. This last equation is the complete expression for $J_{l,s}(P,P')$ when P is any permutation and P' differs from P in the way we have specified. If we were to choose a more complicated pair of permutations that could not be specified in this way then we could not satisfy the s conditions (A.8) on the wave vectors identically.

We next consider the sum for $H_{l,s}$,

$$H_{l,s}=A_lA_l^*\sum_P\sum_{P'}J_{l,s}(P,P'). \tag{A.10}$$

Now since the permutation P' is labeled by the number of pairs of adjacent indices that it permutes we have at once that

$$\sum_{P'}J_{l,s}(P,P')=\sum_{p=0}^{s}{}^sC_pJ_{l,s}(P,p). \tag{A.11}$$

The permutation P is on the other hand labeled by the particular wave vectors that are associated with the coordinates $\mathbf{r}_j$. But $J_{l,s}(P,p)$ depends only on the pairs of wave vectors that are associated with relative coordinates $\varrho_1\cdots\varrho_p$. Therefore all permutations that permute the N indices so that the same wave vectors $\mathbf{k}$ are associated with the coordinates $\varrho_1\cdots\varrho_p$ will lead to the above expression for $J_{l,s}(P,p)$. Since we have $(N-2p)$ wave vectors that do not appear in the expression $J_{l,s}(P,p)$ and these vectors are equal in groups $n_{\mathbf{k}_i}-1$ or $n_{\mathbf{k}_i}$, according as one of the vectors in the group $n_{\mathbf{k}_i}$ appears in $J_{l,s}$ or not, the number of permutations P that lead to the same expression for $J_{l,s}$ is simply

$$(N-2p)!/\prod_{i=1}^{2p}(n_{\mathbf{k}_i}-i)!\prod_{j>2p}(n_{\mathbf{k}_j})!. \tag{A.12}$$

To complete the summation over P we merely have to sum over-all values of the wave vectors in $J_{l,s}$. After a few elementary reductions we get,

$$H_{l,s}=\sum_{p=0}^{s}{}^sC_pV^{-s}K^{s-p}L_l^p(N-2_p)!/N!, \tag{A.13}$$

where we have used the fact that

$$A_lA_l^*=V^{-N}\prod_j(n_{\mathbf{k}j})!/N!,$$

$$K=\int_{\varrho}f(\varrho)d\varrho, \tag{A.16}$$

and

$$L_l=\sum_{\mathbf{k}_1\neq\mathbf{k}_2}\sum n_{\mathbf{k}_1}n_{\mathbf{k}_2}\int_{\varrho}f(\varrho)\exp[2\pi i\varrho\cdot(\mathbf{k}_1-\mathbf{k}_2)]d\varrho. \tag{A.15}$$

Consequently, for large N,

$$H_{l,s}=(N/V)^s[K+L_l/N^2]^s=(I_l)^s, \tag{A.16}$$

and this is the result quoted in the text.

We can now easily see why any pairs of permutations that are such that not all the s conditions (A.8) are fulfilled identically do not contribute significantly to $H_{l,s}$. For if t of these conditions are not satisfied identically then they must be imposed as restrictions on the values that the wave vectors $\mathbf{k}$ can take. Therefore the contribution to $H_{l,s}$ from a permutation of this type will be exactly the same as that given by Eq. (A.16) except that there will be t restrictions on the summations over the $\mathbf{k}$'s. Now since the $n_{\mathbf{k}}$ obey the condition $\sum_{\mathbf{k}}n_{\mathbf{k}}=N$ each restriction we impose on the summations effectively introduces a factor N^{-1} in $H_{l,s}$. If we have t restrictions then we introduce a factor N^{-t} and the contribution to $H_{l,s}$ will therefore be negligible for large N.

APPENDIX B

In this Appendix, we shall show that it is permissible to replace $\langle(I_l)^r\rangle^0$ by $(\langle I_l\rangle^0)^r$ in Eq. (2.27). First we notice that $\langle(I_l)^r\rangle^0=(\langle I_l\rangle^0)^r$, if $r=0$ or 1. Consequently the error introduced into F_1 by this approximation can only depend on second and higher powers of the integral I_l. Let us now write

$$\langle(I_l)^r\rangle^0=(\langle I_l\rangle^0)^r(1+\Delta_r). \tag{B.1}$$

Then it can be easily shown, using the methods developed by Fowler,[14] that

$$|\Delta_r|\leqslant(1+br/N)^r-1\ll(1+b)^r, \tag{B.2}$$

where b is a quantity of order unity. From Eqs. (B.1) and (B.2) together with Eqs. (2.29) and (2.30) of the text, we see that the magnitude of the error, ΔF_1, in F_1 obeys the following inequality

$$|\Delta F_1|\ll N|\langle I_l\rangle^0bkT|, \tag{B.3}$$

and is therefore at most of order N. If we now bear in mind that ΔF_1 can only depend on second and higher powers of I_l then we see that it can be written in the form $Nf(I_l)$, where $f(I_l)$ depends only on second and higher powers of I_l. But any quantity of this order is negligible compared with $N\langle I_l\rangle^0$ and therefore the error introduced into F_1 by this approximation is negligible.

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[14] R. H. Fowler, reference 8, Chap. 20.