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Partition Function for a System of Interacting Bose-Einstein Particles*†

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It is shown by a rigorous development from first principles that a relatively simple form for the partition function of an imperfect Bose-Einstein gas can be obtained. This form is that of a $3N$-dimensional integral (N being the total number of particles) the integrand of which can be completely determined for any given interparticle interaction provided certain, in general small, many-body quantum mechanical effects are ignored. The final evaluation of the partition function in closed form requires that this integrand be approximated by functions sufficiently tractable that the $3N$-dimensional integral can be performed.

I. INTRODUCTION

THE derivation of the thermodynamic properties of a system of ideal (noninteracting) Bose-Einstein particles is well known.[1–3] Treatment of the physical case, however, where interparticle interactions are included, is in general much more difficult and the partition function for such a system has as yet been accurately evaluated only under very special circumstances, e.g., for temperatures sufficiently high that an expansion of the interaction terms in inverse powers of the temperature is rapidly convergent, or for very low densities (virial coefficient expansion).

In this paper we will show, by a rigorous development from first principles, that a relatively quite simple form for the partition function can be obtained. This form is that of a $3N$-dimensional integral (N being the total number of particles) the integrand of which can be completely determined for any given interparticle interaction provided certain, in general small, many-body quantum mechanical effects are ignored. The final evaluation of the partition function in closed form then requires that this integrand be approximated by functions sufficiently tractable that the $3N$-dimensional integration can be performed.

It is seen that the above-mentioned many-body effects contribute only to the long-range density fluctuations discussed, e.g., by Feynman,[4] and are therefore important only for temperatures sufficiently low so that the average particle wavelength is greater than the average interparticle separation. We hope to give a more detailed discussion of these effects in a subsequent publication.

A discussion of the application of these results to the case of He^4 is given in the last section, and a preliminary rather crude model, similar to that recently proposed by Feynman,[5] which approximates to some of the more important features of the partition function in this case, is set up. The results of this model are evaluated in the succeeding paper (hereafter called II).

II. DEFINITIONS OF THE PARTITION FUNCTION

The partition function to be evaluated is defined by

$$Z=\sum_j \exp(-\beta U_j), \tag{1}$$

where $\beta=1/kT$, and U_j are the energy levels of the system. This may, alternatively, be written as the Slater sum:

$$Z=\sum_\alpha(\Psi_\alpha, \exp-\{\beta(H_0+H')\}\Psi_\alpha), \tag{2}$$

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[1] A. Einstein, Ber. Berl. Akad. 261 (1924); 3 (1925).

[2] F. London, Phys. Rev. **54**, 947 (1938).

[3] B. Kahn and G. E. Uhlenbeck, Physica **5**, 399 (1938).

[4] R. P. Feynman, Phys. Rev. **91**, 1301 (1953).

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

where H_0 is the kinetic energy operator for the N-particles, H' is the interaction energy of the complete system, and the Ψ_α are any *appropriately symmetrized* wave functions which form a complete and orthonormal set over the volume of the container of the system.

Equation (2) is, of course, quite general irrespective of the type of statistics holding. The wave functions Ψ_α must merely be chosen in accord with whatever statistics are being dealt with. In this paper we will be concerned exclusively with Bose-Einstein statistics. For this case it is easy to show that (2) takes the form

$$Z=(1/N!)\sum_P\sum_j(\Phi_j^P,\ \exp\{-\beta(H_0+H')\}\Phi_j),\quad (3)$$

where N is the number of particles in the system, and the Φ_j are any complete and normalized set of *unsymmetrized* (Boltzmann) wave functions. The symbol P denotes some permutation of the set of coordinates $\mathbf{r}_1, \mathbf{r}_2, \cdots \mathbf{r}_N$ of the particles, and $\sum_P$ implies a summation over all permutations. Thus Φ_j^P is the same as Φ_j except that a certain interchange of coordinates is effected by the P. Because of the summation on P any set of wave functions Φ_j for a Boltzmann system is permissible—it is irrelevant in which way the wave functions describing states of the same energy, for example, are constructed.

Equation (3) forms our starting point for evaluation of Z.

III. EVALUATION OF THE PARTITION FUNCTION

In this section, we discuss the question of the evaluation of (3). We will first consider very briefly the case of the ideal gas, since the form then taken by (3) will be interesting for the purpose of comparison when we come to interacting systems.

1. Perfect Gas

Here we may write

$$\Phi_j=\frac{1}{(V)^{N/2}}\exp\left(\frac{i}{\hbar}\sum_{k=1}^{N}\mathbf{p}_k\cdot\mathbf{r}_k\right),\quad (4)$$

$$\Phi_j=\frac{1}{(V)^{N/2}}\exp\left(\frac{i}{\hbar}\mathbf{p}\cdot\mathbf{r}\right),\quad (4a)$$

the state j now referring to a particular set of the momenta $\mathbf{p}_1, \cdots \mathbf{p}_N$. In (4a) we introduce, for convenience of notation, the $3N$-dimensional vectors $\mathbf{p}$ and $\mathbf{r}$.

If we insert this in (3), and replace the summation over Boltzmann states j by an integration over momenta, i.e.,

$$\sum_j\rightarrow\frac{V^N}{(2\pi\hbar)^{3N}}\int d\mathbf{p},$$

we find, after integrating over the momenta, that

$$Z=\frac{1}{N!}\frac{1}{\lambda^{3N}}\sum_P\int_V d\mathbf{r}\exp\left\{-\frac{\pi}{\lambda^2}(\mathbf{r}-\mathbf{r}_P)^2\right\}.\quad (5)$$

Here

$$\lambda^2=2\pi\hbar^2\beta/m,\quad (6)$$

and $\mathbf{r}_P$ is that position vector which replaces $\mathbf{r}$ in the permutation P.

This is the partition function as obtained by Kahn and Uhlenbeck[3] and yields the well-known properties of the perfect gas, including the Bose-Einstein condensation. The replacement of the summation over the states of the Boltzmann system by an integration is a legitimate procedure as long as the subsequent integration over coordinates is correctly limited by the volume of the container.[6]

2. Interacting Particles

Because of the simplicity of the wave functions (4) it is tempting to try to evaluate (3) in the general case also by continuing to choose the Φ_j to be plane waves. The difficulty then is clearly the evaluation of exp $\times\{-\beta(H_0+H')\}\Phi_j$.

Two methods which have been developed to tackle this problem may be summarized as follows: Let us introduce an operator $S(\beta)$ such that

$$\exp\{-\beta(H_0+H')\}=S(\beta)\exp(-\beta H_0).\quad (7)$$

Then the operation of $\exp(-\beta H_0)$ on Φ_j is trivial [assuming the Φ_j to be plane waves—Eq. (4)]. In order to evaluate $S(\beta)$, we note that this operator must satisfy the equation:

$$\partial S/\partial\beta=-S(\beta)H'(\beta),\quad (8)$$

where

$$H'(\beta)=\exp(-\beta H_0)H'\exp(+\beta H_0).$$

Equation (8) is subject, of course, to the boundary condition $S\rightarrow 1$ as $\beta\rightarrow 0$.

Equation (8) may now be solved by an iteration procedure in a manner familiar from electrodynamics and yields for S the ordered exponential:

$$S(\beta)=1+\sum_{n=1}^{\infty}(-1)^n\int_0^{\beta}d\beta_1\int_0^{\beta_1}d\beta_2\cdots\int_0^{\beta_{n-1}}\times d\beta_n H'(\beta_n)\cdots H'(\beta_1).\quad (9)$$

Moreover, it is possible to carry out the operation of each term of (9) on the plane-wave Φ_j's.

This expression, derived by Goldberger and Adams,[7] is of use however only at temperatures sufficiently high that the interaction involved in H' can be considered as weak. It is essentially an expansion in powers of the ratio of the potential to kinetic energies. But in most physical systems of interest the interaction between

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[6] Kahn and Uhlenbeck (reference 3) actually let these limits be infinite, but devise a prescription for obtaining the partition function below the condensation point. When the true limits of integration are retained, however, the evaluation of the integral (5) yields a form for the partition function identical to that obtained by London (reference 2), and the thermodynamic properties both above and below the transition point can immediately be derived (see Appendix, paper II).

[7] M. L. Goldberger and E. N. Adams, J. Chem. Phys. **20**, 240 (1952).

particles is extremely strong (e.g., very strongly repulsive at short distances) and it is hopeless to attempt to employ (9) at anything but high temperatures.

Another approach is to note that, instead of (8), an alternative equation for S is

$$\partial S/\partial\beta=-H'S(\beta)+[S(\beta),H_0], \qquad (10)$$

where $[\,]$ signifies that the commutator be taken. If now (10) be solved by iteration, the first step being to ignore the commutator of S and H_0 on the right-hand side, we obtain

$$S(\beta)=\exp(-\beta H')\left\{1+\int_0^\beta d\beta_1 \right.$$
$$\left.\times\{H_0-\exp(+\beta_1 H')H_0\exp(-\beta_1 H')\}+\cdots\right\}. \qquad (11)$$

Here we have derived the semiclassical expansion of Wigner[8]—as extended by Mayer and Band.[9] The consequences of the first term of (11) have, of course, been studied by many workers, particularly as applied to He^4 (e.g., Matsubara[10]). As we will see later, this term gives Z accurately for temperatures sufficiently high that $\lambda\ll r_0$, where r_0 is the range of the interparticle interaction. In the case of He^4, for example, this means temperatures >80°K.

The evaluation of higher terms in (11), operating on the plane-wave Φ_j's, can in principle be carried out. However, they become prohibitively complicated after the first two or three. But a very large number of terms of (11) become important at the low temperatures of so much physical interest (e.g., the vicinity of the λ-transition in He^4). The expansion (11) cannot be employed therefore for a study of this low-temperature region.

The method which we will now develop differs radically from the above approaches. Rather than expanding in an infinite series and being troubled by convergence problems, we will deal with an infinite product which may be employed for evaluation of the partition function not only for high temperatures but also for low.

Let us write

$$\exp\{-\beta(H_0+H')\}=\lim_{n\to\infty}[\exp(-\beta H'/n)\exp(-\beta H_0/n)]^n$$
$$=\lim_{n\to\infty}\exp(-\beta H'/n)\exp(-\beta H_0/n)$$
$$\times\exp(-\beta H'/n)\cdots\exp(-\beta H_0/n). \qquad (12)$$

We also make use of the theorem, established in the Appendix, that (we retain the $3N$-dimensional vector notation):

$$\exp(-\beta H_0/n)f(\mathbf{r})=\frac{1}{\lambda_n^{3N}}\int d\boldsymbol{\delta}\exp\left(-\frac{\pi}{\lambda_n^2}\delta^2\right)$$
$$\times f(\mathbf{r}-\boldsymbol{\delta}), \qquad (13)$$

where $\lambda_n^2=\lambda^2/n$. Thus the effect of the operator $\exp(-\beta H_0/n)$ is merely to "smear" or average the function $f(\mathbf{r})$ over small displacements of each coordinate by amounts $\gtrsim\lambda_n$.

On substituting (12) in (3), making use of (13), and performing the integration over momenta exactly as in the case of the perfect gas, we obtain for the partition function:

$$Z=\lim_{n\to\infty}\frac{1}{N!}\frac{1}{\{\lambda_n^{3N}\}^n}\sum\nolimits_P\int_V d\mathbf{r}d\boldsymbol{\delta}^{(1)}d\boldsymbol{\delta}^{(2)}\cdots d\boldsymbol{\delta}^{(n-1)}$$
$$\times\exp\left\{-\frac{\pi}{\lambda_n^2}(\mathbf{r}-\mathbf{r}_P-\boldsymbol{\delta}^{(1)}-\boldsymbol{\delta}^{(2)}\cdots\boldsymbol{\delta}^{(n-1)})\right\}^2$$
$$\times\exp\left\{-\frac{\pi}{\lambda_n^2}\sum_{\nu=1}^{n-1}(\delta^{(\nu)})^2\right\}V_n(\mathbf{r})V_n(\mathbf{r}-\boldsymbol{\delta}^{(1)})$$
$$\times V_n(\mathbf{r}-\boldsymbol{\delta}^{(1)}-\boldsymbol{\delta}^{(2)})\cdots$$
$$\times V_n(\mathbf{r}-\boldsymbol{\delta}^{(1)}-\boldsymbol{\delta}^{(2)}\cdots\boldsymbol{\delta}^{(n-1)}). \qquad (14)$$

Here we have let

$$V_n(\mathbf{r})=\prod_{i>j}\exp[-\beta\mathcal{V}(r_{ij})/n],$$

$\mathcal{V}$ denoting the interaction between any two particles.

By completing the squares on the $\boldsymbol{\delta}$'s in the exponential of (14) and transforming to the resulting variables of integration, this equation now becomes

$$Z=\frac{1}{N!}\frac{1}{\lambda^{3N}}\sum\nolimits_P\int_V d\mathbf{r}\exp\left\{-\frac{\pi}{\lambda^2}(\mathbf{r}-\mathbf{r}_P)\right\}^2 Q(\mathbf{r},\mathbf{r}_P), \qquad (15)$$

where

$$Q(\mathbf{r},\mathbf{r}_P)=\lim_{n\to\infty}\frac{1}{\{\lambda_n^{3N}\}^{(n-1)}}\int d\boldsymbol{\delta}^{(1)}\cdots$$
$$\times d\boldsymbol{\delta}^{(n-1)}\exp\left\{-\frac{\pi}{\lambda_n^2}\sum_{\nu=1}^{n-1}(\delta^{(\nu)})^2\right\}V_n\left\{\mathbf{r}-A_1(\mathbf{r}-\mathbf{r}_P)\right.$$
$$-(1/2^{\frac{1}{2}})\boldsymbol{\delta}^{(1)}-\tfrac{1}{2}(\tfrac{2}{3})^{\frac{1}{2}}\boldsymbol{\delta}^{(2)}\cdots-\tfrac{1}{3}(\tfrac{3}{4})^{\frac{1}{2}}\boldsymbol{\delta}^{(3)}$$
$$\left.-\frac{1}{(n-1)}\left(\frac{n-1}{n}\right)^{\frac{1}{2}}\boldsymbol{\delta}^{(n-1)}\right\}V_n\left\{\mathbf{r}-A_2(\mathbf{r}-\mathbf{r}_P)\right.$$
$$\left.-(\tfrac{2}{3})^{\frac{1}{2}}\boldsymbol{\delta}^{(2)}-\tfrac{2}{3}(\tfrac{3}{4})^{\frac{1}{2}}\boldsymbol{\delta}^{(3)}\cdots-\frac{2}{(n-1)}\left(\frac{n-1}{n}\right)^{\frac{1}{2}}\boldsymbol{\delta}^{(n-1)}\right\}$$
$$\cdots$$
$$\times V_n\left\{\mathbf{r}-A_{n-1}(\mathbf{r}-\mathbf{r}_P)-\left(\frac{n-1}{n}\right)^{\frac{1}{2}}\boldsymbol{\delta}^{(n-1)}\right\}V_n(\mathbf{r}). \qquad (16)$$

Here the coefficients A_m are given by the series:

$$A_m=m\sum_{\mu=0}^{n-1-m}\frac{1}{(\mu+m)(\mu+m+1)}=\left(1-\frac{m}{n}\right). \qquad (17)$$

We see that in Eq. (15) we have an exact expression for Z which is of a form very similar to the first term of the semiclassical expansion—Eq. (11). Indeed the partion function (15) is the same as that of a "classical" Bose-Einstein gas, with an equivalent temperature-dependent interaction (which actually includes some many-body forces—see later). When n is taken to be merely unity, (15) is precisely the "classical" result.

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[8] E. P. Wigner, Phys. Rev. **40**, 749 (1932).

[9] J. Mayer and W. Band, J. Chem. Phys. **15**, 191 (1947).

[10] T. Matsubara, Progr. Theoret. Phys. (Japan) **6**, 714 (1951).

Also in the limit of no interaction ($V_n=1$), we have $Q=1$ and (15) immediately passes into (5).

We shall now show that, on the basis of an approximation which is justified at all temperatures except those very close to absolute zero, (16) can be put in a form which enables Q to be evaluated for any given interparticle interaction.

Consider first, for simplicity, the evaluation of Q when $\mathbf{r}_P\equiv\mathbf{r}$ [the identity permutation $P=1$ (say)]. Let us go through the steps by which $Q_{P=1}$ would be calculated. The first operation is that of "smearing" the function $V_n(\mathbf{r})$, i.e., (we forego the $3N$-dimensional notation here) we have to perform

$$\frac{1}{\lambda_n^{3N}}\int d\boldsymbol{\delta}_1\cdots d\boldsymbol{\delta}_N\prod_{\mu}\exp\left(-\frac{\pi}{\lambda_n^2}\boldsymbol{\delta}_\mu^2\right)\times\prod_{i>j}v_n\left(\left|\mathbf{r}_{ij}-\frac{1}{\sqrt{2}}\boldsymbol{\delta}_{ij}\right|\right),\tag{18}$$

where

$$\mathbf{r}_{ij}=\mathbf{r}_i-\mathbf{r}_j,\quad \boldsymbol{\delta}_{ij}=\boldsymbol{\delta}_i-\boldsymbol{\delta}_j,$$

and

$$v_n(\mathbf{r}_{ij})=\exp\{-\beta\mathcal{V}(\mathbf{r}_{ij})/n\}.$$

Now since we are interested in the limit $n\rightarrow\infty$ (i.e., $\lambda_n\rightarrow 0$), it is correct to expand the function v_n of (18) to second order in the δ's. On omitting terms which vanish on integration, (18) then becomes

$$\begin{aligned}&\frac{1}{\lambda_n^{3N}}\{\prod_{i>j}v_n(r_{ij})\}\int d\boldsymbol{\delta}_1\cdots d\boldsymbol{\delta}_N\left\{\prod_{\mu}\exp\left(-\frac{\pi}{\lambda_n^2}\delta_\mu^2\right)\right\}\\&\quad\times\left[1+\tfrac{1}{2}\sum_{i>j}\frac{\delta_{ij}^2}{2!}\frac{\nabla^2v_n(r_{ij})}{v_n(r_{ij})}+\tfrac{1}{2}\sum_{i>j>k}\frac{\{\boldsymbol{\delta}_{ij}\cdot\boldsymbol{\nabla}v_n(r)_{ij}\}\boldsymbol{\delta}_{jk}\cdot\boldsymbol{\nabla}v_n(r_{jk})}{v_n(r_{ij})v_n(r_{jk})}\right]\\&=\{\prod_{i>j}v_n(r_{ij})\}\left[1+\frac{3}{4\pi}\lambda_n^2\sum_{i>j}\frac{\nabla^2v_n(r_{ij})}{v_n(r_{ij})}-\frac{1}{4\pi}\lambda_n^2\sum_{i>j>k}\frac{\boldsymbol{\nabla}v_n(r_{ij})\cdot\boldsymbol{\nabla}v_n(r_{jk})}{v_n(r_{ij})v_n(r_{jk})}\right].\end{aligned}\tag{19}$$

The second and third terms of (19) give the changes which have been affected by the operation $\exp(-\beta H_0/n)$ on the function $\prod v_n$. The third term represents three-body interactions, and shows that the final form for Q must involve many-body interactions of all orders up to N. However, on writing this term of (19) in the form

$$-\frac{\lambda_n^2}{4\pi}\{\prod_{i>j}v_n(r_{ij})\}\sum_{i>j>k}\frac{\mathbf{r}_{ij}\cdot\mathbf{r}_{jk}}{r_{ij}r_{jk}}\times\frac{\{[dv_n(r_{ij})/dr_{ij}]\times[dv_n(r_{jk})/dr_{jk}]\}}{v_n(r_{ij})v_n(r_{jk})},$$

we see that it should be small compared to the second (two-body) correction term of (19) provided we can assume the end result that the most probable distribution of particles in the gas[11] is one of uniformity throughout the container. In this event, those particles which are interacting with any given particle are on the average symmetrically disposed around this particle, and (14) would depend on fluctuations from this average for its contributions. It should therefore be much less important than the second term of (19), in which all terms of the summation are additive for the average distribution.

If we assume, therefore, that for physical systems of interest the third term of (19) is unimportant, we then find that, to second order in the expansion of v_n, (18) is identical to the expression

$$\frac{1}{(\lambda_n^3)^{N(N-1)/2}}\prod_{i>j}\left\{\int d\boldsymbol{\delta}\exp\left(-\frac{\pi}{\lambda_n^2}\delta^2\right)v_n(|\mathbf{r}_{ij}-\boldsymbol{\delta}|).\right.\tag{20}$$

Thus, on the foregoing approximation, the result of operation (18) is again a product of the form

$$\prod_{i>j}v_n'(r_{ij}).$$

In this manner we can work right through expression (16). We have, then, that

$$Q_{P=1}=\prod_{i>j}q(r_{ij}),\tag{21}$$

$$\begin{aligned}q(r_{ij})=\lim_{n\to\infty}&\frac{1}{\{\lambda_n^3\}^{(n-1)}}\int d\boldsymbol{\delta}_{ij}^{(1)}\cdots d\boldsymbol{\delta}_{ij}^{(n-1)}\exp\left\{-\frac{\pi}{\lambda_n^2}\sum_{\nu=1}^{n-1}(\delta_{ij}^{(\nu)})^2\right\}\\&\times v_n\left\{\mathbf{r}_{ij}-\sqrt{2}\left[\frac{1}{\sqrt{2}}\boldsymbol{\delta}_{ij}^{(1)}+\tfrac{1}{2}(\tfrac{2}{3})^{\frac{1}{2}}\boldsymbol{\delta}_{ij}^{(2)}+\cdots\frac{1}{n-1}\left(\frac{n-1}{n}\right)^{\frac{1}{2}}\boldsymbol{\delta}_{ij}^{(n-1)}\right]\right\}\\&\times v_n\left\{\mathbf{r}_{ij}-\sqrt{2}\left[(\tfrac{2}{3})^{\frac{1}{2}}\boldsymbol{\delta}_{ij}^{(2)}+\tfrac{2}{3}(\tfrac{3}{4})^{\frac{1}{2}}\boldsymbol{\delta}_{ij}^{(3)}+\cdots\frac{2}{n-1}\left(\frac{n-1}{n}\right)^{\frac{1}{2}}\boldsymbol{\delta}_{ij}^{(n-1)}\right]\right\}\\&\qquad\cdots\\&\times v_n\left\{\mathbf{r}_{ij}-\sqrt{2}\left[\left(\frac{\nu}{\nu+1}\right)^{\frac{1}{2}}\boldsymbol{\delta}_{ij}^{(\nu)}+\frac{\nu}{\nu+1}\left(\frac{\nu+1}{\nu+2}\right)^{\frac{1}{2}}\delta_{ij}^{(\nu+1)}+\cdots\frac{\nu}{n-1}\left(\frac{n-1}{n}\right)^{\frac{1}{2}}\boldsymbol{\delta}_{ij}^{(n-1)}\right]\right\}\\&\qquad\cdots\\&\times v_n\left\{\mathbf{r}_{ij}-\sqrt{2}\left(\frac{n-1}{n}\right)^{\frac{1}{2}}\boldsymbol{\delta}_{ij}^{(n-1)}\right\}v_n(\mathbf{r}_{ij}).\end{aligned}\tag{22}$$

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[11] That is that distribution which contributes most to the integral of (15).

Although the limit of n going to infinity has to be taken to get $q(r_{ij})$ exactly, in practice it is possible to choose a sufficiently large but finite n such that q is obtained to a desired accuracy. Even so, the amount of numerical work necessary to evaluate $q(r_{ij})$ from (22) is, of course, extremely large. For this purpose, however, the following approximation to (22) is quite adequate:

$$
\begin{aligned}
q(r_{ij}) \simeq \lim_{n\to\infty} & \frac{1}{(\lambda_n{}^3)^{(n-1)}} \int d\boldsymbol{\delta}_{ij}{}^{(1)} \cdots d\boldsymbol{\delta}_{ij}{}^{(n-1)} \exp\left\{-\frac{\pi}{\lambda_n{}^2} \sum_{\nu=1}^{n-1} (\delta_{ij}{}^{(\nu)})^2\right\} \\
& \times v_n\left\{\mathbf{r}_{ij} - \sqrt{2}\left[\frac{1}{\sqrt{2}}\boldsymbol{\delta}_{ij}{}^{(1)} + (\tfrac{2}{3})^{\frac{1}{2}}\boldsymbol{\delta}_{ij}{}^{(2)} + \cdots\right]\right\} \\
& \times v_n\{\mathbf{r}_{ij} - \sqrt{2}[(\tfrac{2}{3})^{\frac{1}{2}}\boldsymbol{\delta}_{ij}{}^{(2)} + (\tfrac{3}{4})^{\frac{1}{2}}\boldsymbol{\delta}_{ij}{}^{(3)} + \cdots]\} \\
& \cdots \\
& \times v_n\left\{\mathbf{r}_{ij} - \sqrt{2}\left[\left(\frac{\nu}{\nu+1}\right)^{\frac{1}{2}}\boldsymbol{\delta}_{ij}{}^{(\nu)} + \left(\frac{\nu+1}{\nu+2}\right)^{\frac{1}{2}}\boldsymbol{\delta}_{ij}{}^{(\nu+1)} + \cdots\right]\right\} \\
& \cdots \\
& \times v_n\left\{\mathbf{r}_{ij} - \sqrt{2}\left(\frac{n-1}{n}\right)^{\frac{1}{2}}\boldsymbol{\delta}_{ij}{}^{(n-1)}\right\} v_n(\mathbf{r}_{ij}). \qquad (23)
\end{aligned}
$$

The reason for this is that in each v_n of Eqs. (22) or (23) only the first few "smearing" variables $\boldsymbol{\delta}_{ij}{}^{(\nu)}$ are important, and (except for the very first v_n) it is largely irrelevant whether the smearing variables[12] are the square-bracketed terms of Eqs. (22) or (23).

Thus, from Eq. (23), q may be evaluated by performing $(n-1)$ operations of the form

$$\frac{1}{\lambda_n{}^3}\int d\boldsymbol{\delta} \exp\left\{-\frac{\pi}{\lambda_n{}^2}\delta^2\right\} f(|\mathbf{r}_{ij} - \alpha\boldsymbol{\delta}|). \qquad (24)$$

For the first step the function f is to be merely v_n. The integral (24) (with $\alpha = 1$) then yields a new function which is to be multiplied by v_n and again averaged by the integration of (24) [with α now $(4/3)^{\frac{1}{2}}$] and so on. After $(n-1)$ such steps have been performed, we multiply for the last time by $v_n(r_{ij})$ to get q.

For a given interaction and temperature, therefore, q can be obtained by performing n numerical integrations for each value of the argument r_{ij}. [The angle integrations of (24) are done analytically.] We note that, in computing q for a certain low temperature T/n, the various steps involved also give it for the temperatures T, $T/2$, $T/3 \cdots T/n$.

A convenient way of obtaining an estimate of the accuracy involved by using a certain number of steps n is the following: instead of (12) we could equally well write:

$$\exp\{-\beta(H_0 + H')\} = \lim_{n\to\infty}\left[\exp\left(-\frac{\beta}{n}H_0\right) \times \exp\left(-\frac{\beta}{n}H'\right) \cdots \exp\left(-\frac{\beta}{n}H'\right)\right]. \qquad (25)$$

Equation (25) gives precisely the same results as (12) except that in obtaining q one more smearing process [Eq. (22)] is performed after multiplying by the last v_n. Thus n should be sufficiently large that the difference between the two results obtained by carrying out the nth smearing and not doing so can be tolerated. Computations which we have performed indicate that the two curves thus obtained for q actually bracket the true curve, and of course tend closer to each other the larger n.

In the case of the general function Q, precisely the same considerations apply in expressing it in the form

$$Q = \prod_{i>j} q_P(\mathbf{r}_{ij}, \mathbf{r}_{ij}{}^P), \qquad (26)$$

where

$$q_P(\mathbf{r}_{ij}, 0) = q(r_{ij}).$$

Also, even when $\mathbf{r}_{ij} \neq \mathbf{r}_{ij}{}^P$, $q_P(\mathbf{r}_{ij}, \mathbf{r}_{ij}{}^P)$ may be evaluated by going through the same steps described above for obtaining $q(r_{ij})$ from Eq. (23). Much more numerical work is now required, of course, since $(n-1)$ integrations have to be performed not only for various values of $\mathbf{r}_{ij}$, but also for various values of both $\mathbf{r}_{ij}{}^P$, and the angle between $\mathbf{r}_{ij}$ and $\mathbf{r}_{ij}{}^P$.[13] Once this has been carried

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[12] Indeed, for all actual calculations which have been performed, the results for q obtained by taking only the first δ variable in each v_n differs very little from the results obtained from Eq. (23). For example, curves which are given in the next section for the case of He^4, obtained from Eq. (23) have the heights of their maxima above unity increased by less than 20 percent, when computed by the above much cruder approximation. The actual curve will lie between the two results, and should be much closer to the results of (23).

[13] This work is not necessary if $\lambda/\sqrt{\pi}$ is considerably less than the range r_0 of $\mathcal{V}$; in this event the added arguments $A_m(\mathbf{r}_{ij} - \mathbf{r}_{ij}{}^P)$ will produce only a small smearing effect to $q(r_{ij})$ and may be ignored.

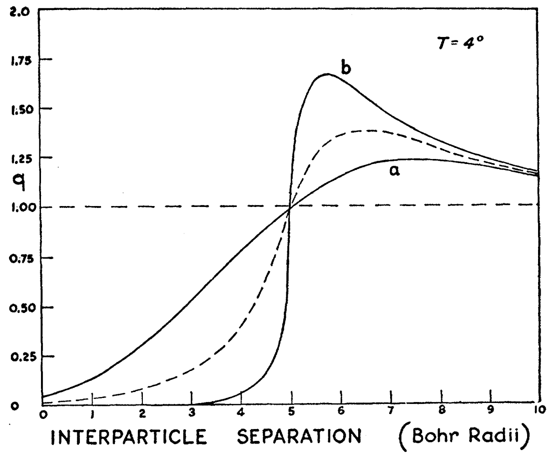

FIG. 1. Curves of $q(r_{ij})$ for $T=4°$, computed by taking $n=5$. Curve (*b*) is that obtained when the last smearing is not performed, and curve (*a*) is that obtained from (b) by performing the last smearing process. The dotted curve is a compromise between (*a*) and (*b*), estimating the actual behavior of q.

out for a given interaction $\mathcal{V}$ however, the Q of (15) is completely known.

A more detailed discussion of the many-body quantum-mechanical effects which are ignored in the above will be made in a subsequent publication. It will be shown that they are associated with the long range density fluctuations, which are important only for temperatures such that $\lambda/2\sqrt{\pi}\gtrsim r_a$, where r_a is the average interparticle spacing.

III. APPLICATION TO He^4

In this section we give a preliminary discussion of the application of our results to the case of He^4 at low temperatures. We have made numerical calculations of the function $q(r_{ij})$ for this case, the interaction $\mathcal{V}$ used being that of Slater and Kirkwood.[14,15] The magnitude of each of the steps used was such that β/n corresponded to a temperature of 20°. Thus, for example, 5 steps were taken for $T=4°$, 10 for $T=2°$, and 20 for $T=1°$.

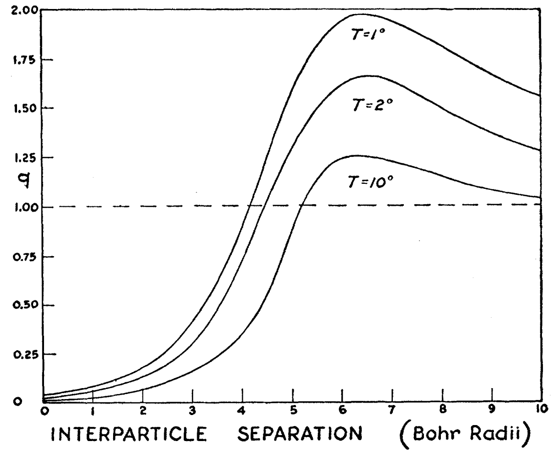

FIG. 2. Curves of $q(r_{ij})$ for a number of temperatures.

In Fig. 1 we see the behavior thus found for $q(\mathbf{r}_{ij})$ at $T=4°$. Curve (*b*) is that obtained when the last smearing is not performed, and this passes into curve (*a*) by means of the last smearing process. The differences between the two curves show that, for a really precise determination of $q(r_{ij})$ at all points, we should have taken smaller intervals β/n. These curves are adequate for our present discussion, however, and we consider the actual behavior of $q(r_{ij})$ to be not far from a compromise between (*a*) and (*b*), such as the dotted curve.

Similar compromise curves for a number of other temperatures are given in Fig. 2.

It is interesting to see what a vast improvement is obtained by using the above rather small number of steps over the crudest approximation of using only one step ($n=1$). At 4° the two curves for $n=1$ are shown in Fig. 3, (*a*) being the unsmeared and (*b*) the smeared curve. It is seen that the two are completely different from each other, and allow of no reasonable estimate of the actual behavior of $q(r_{ij})$. With increase of n from 1 to 5, however, these two curves pass into those of Fig. 1.

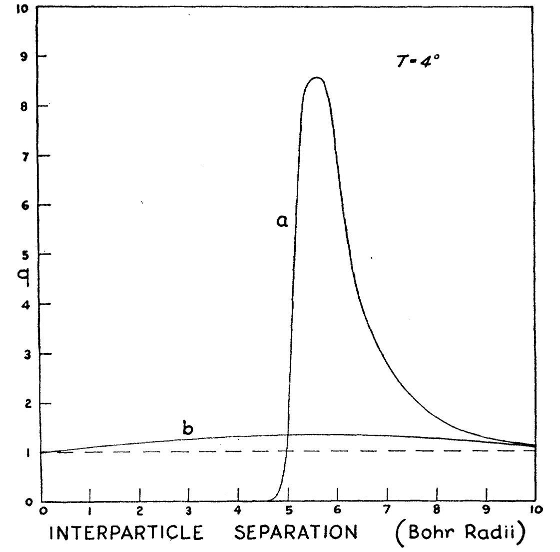

FIG. 3. The curves obtained for q at $T=4°$ when $n=1$, (*a*) being the unsmeared and (*b*) the smeared curve. The differences between these curves and those of Fig. 1 are to be noted.

In this connection it is worthwhile to note how incorrect it is at these low temperatures to neglect all quantum-mechanical effects other than the statistics—i.e., to use only the first term of (11). This would give the result

$$q(r_{ij})=\exp\{-\beta\mathcal{V}(r_{ij})\}. \tag{27}$$

At 4° this is just the curve (*a*) of Fig. 3 which differs radically from the actual curve of Fig. 1. The differ-

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[14] J. C. Slater and J. G. Kirkwood, Phys. Rev. **37**, 682 (1931).

[15] The precise behavior of $\mathcal{V}$ for small interparticle distances (<2 Bohr radii) was found to be completely irrelevant to our results as long as it remained strongly repulsive.

ence is even more pronounced for lower temperatures. At 2° for example (i.e., the vicinity of the λ transition) Eq. (25) would give a peak due to the attractive portion[14] of $\mathcal{V}$ of order of magnitude 100, instead of about 1.8 (Fig. 2).

The curves of Figs. 1 and 2 show clearly the characteristics of the function $q(r_{ij})$. Its most important property is that, at the low temperatures being considered, it is always very small for small interparticle separation. Thus the contribution to (15) from configurations in which two or more particles (whose coordinates are unaffected by the permutation P) are close together will be quite small.

It can easily be seen that the general function $q_P(\mathbf{r}_{ij},\mathbf{r}_{ij}{}^P)$ for $\mathbf{r}_{ij}{}^P \neq \mathbf{r}_{ij}$ also behaves in the above manner as a function of r_{ij}. The fact that for all the final steps of (16) the coefficients A_m [Eq. (17)] are very small ensures that $q_P(\mathbf{r}_{ij},\mathbf{r}_{ij}{}^P)$ has the same qualitative behavior as a function of r_{ij} as $q(r_{ij})$. We now have merely that the precise *small* value of q_P for small r_{ij} is dependent on $\mathbf{r}_{ij}{}^P$, and also that the precise height of the subsequent rise above unity is dependent on $\mathbf{r}_{ij}{}^P$.

A very simple model which approximates the above features is to ignore the difference between $q_P(\mathbf{r}_{ij},\mathbf{r}_{ij}{}^P)$ and $q(r_{ij})$, and to replace $q(r_{ij})$ by a step function which is zero for all r_{ij} up to some distance r_0, and unity thereafter.[16] The results of this model are evaluated in II, r_0 being taken to be $3.3a_0$ (where a_0 is the Bohr radius). It will be seen in II that (15) then yields a Bose-Einstein condensation point in quite good agreement with the λ-point of liquid helium. Moreover, the thermodynamic properties in the vicinity of the transition point are similar to those observed experimentally for liquid helium.

Of course in ignoring as it does the effect of the attractive part of $\mathcal{V}$, exhibited in $q(r_{ij})$ as a rise above unity in the vicinity of $7a_0$, the above model does not yield the normal gas-liquid transition, and speaks of a gas rather than a liquid at the low temperatures. We consider it very probable that the remaining differences between the results of II and experiment are due to this neglect.

Since it is possible to numerically evaluate $q_P(\mathbf{r}_{ij},\mathbf{r}_{ij}{}^P)$ very accurately by the methods of Sec. III, however, it should be possible for the finer details to be calculated. What is required for this is that a function be found which simulates the behavior of $q_P(\mathbf{r}_{ij},\mathbf{r}_{ij}{}^P)$ in some detail but which is still sufficiently tractable for the integral of (15) to be evaluated. This question is being investigated.

The authors are indebted to Professor Bethe, Professor Dyson, Professor Placzek, and Professor Salpeter for discussions on the subject of this paper.

APPENDIX

We wish to prove Eq. (13), *viz.*,

$$\exp\left(-\frac{\beta}{n}H_0\right)f(\mathbf{r})=\frac{1}{\lambda_n{}^{3N}}\int d\boldsymbol{\delta}\,\exp\left(-\frac{\pi}{\lambda_n{}^2}\right)f(\mathbf{r}-\boldsymbol{\delta}).$$

Let

$$f(\mathbf{r})=\int d\mathbf{k}g(\mathbf{k})\,\exp(i\mathbf{k}\cdot\mathbf{r}).$$

Then

$$\exp\left(-\frac{\beta}{n}H_0\right)f(\mathbf{r})=\int d\mathbf{k}g(\mathbf{k})\,\exp(i\mathbf{k}\cdot\mathbf{r})\,\exp\left(-\frac{\lambda_n{}^2}{4\pi}k^2\right).$$

On introduction of the new variables $\mathbf{q}$ and $\mathbf{R}$ this may be written

$$\frac{1}{(2\pi)^{3N}}\int d\mathbf{R}d\mathbf{q}d\mathbf{k}g(\mathbf{k})\,\exp\left(-\frac{\lambda_n{}^2}{4\pi}q^2\right)\exp(i\mathbf{q}\cdot\mathbf{r})$$

$$\times\exp\{i\mathbf{R}\cdot(\mathbf{k}-\mathbf{q})\}=\frac{1}{\lambda_n{}^{3N}}\int d\mathbf{R}d\mathbf{k}g(\mathbf{k})\,\exp(i\mathbf{k}\cdot\mathbf{R})$$

$$\times\exp\left\{-\frac{\pi}{\lambda_n{}^2}(\mathbf{r}-\mathbf{R})^2\right\}=\frac{1}{\lambda_n{}^{3N}}\int d\mathbf{R}f(\mathbf{R})$$

$$\times\exp\left\{-\frac{\pi}{\lambda_n{}^2}(\mathbf{r}-\mathbf{R})^2\right\}.$$

On changing the variable of integration from $\mathbf{R}$ to $\boldsymbol{\delta}=\mathbf{r}-\mathbf{R}$, we immediately obtain Eq. (13).

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[16] Equation (15) is then very similar to the form for Z recently proposed by Feynman (see reference 5).