TABLE II. Transmitted distribution.

μ	$\dot{N}(\epsilon;\mu;\tau)$	$\dot{N}^0(\epsilon;\mu;\tau)$	$N'(\epsilon;\mu;\tau)$
0	0.33754	0.33840	0.31152
0.05	0.23815	0.23807	
0.1	0.14965	0.14970	
0.2	0.08460	0.08460	0.07788
0.4	0.04003	0.04006	
0.6	0.03064	0.03069	
0.8	0.02325	0.02326	
1	0.01872	0.01873	0.01724

distributions. This enables us, however, to determine the scattering kernel directly from the data. It is not necessary in this method to separate the once-scattered and multiply scattered contributions to compute the scattering kernel[4] and it means that no prior information on the scattering kernel is needed.

Admittedly, the one-speed case which was treated numerically is a very simple one. Nevertheless, in view of the good results in this case, one may expect the present method to be useful also for more realistic and complicated scattering kernels.

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†On leave from the University of Ljubljana, Yugoslavia.

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Exact Inversion of the Fugacity-Density Relation for Ideal Quantum Gases

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The fugacities of ideal Fermi and Bose gases are calculated explicitly as a function of density and temperature, using the analytic properties of the integral appearing in the fugacity-density equation. The Hilbert problem of the theory of analytic functions is encountered.

The equation of state of an ideal Fermi or Bose gas may be stated in terms of two equations with the fugacity (or equivalently chemical potential) left to be eliminated. Appropriate expansions yielding the equation of state in both the high-temperature-low-density and low-temperature-high-density limits are well known for the Fermi case, while in the Bose case additional expansions about the transition point are available. In this paper we calculate the fugacity in both cases explicitly for all densities and temperatures by using the analytic properties of the integral appearing in the fugacity-density equation.

IDEAL FERMI GAS

In the Fermi case, the equation of state is obtained by eliminating the fugacity z from the following equations[1]

$$P/kT=\lambda^{-3}f_{5/2}(z), \tag{1}$$

$$v^{-1}=\lambda^{-3}f_{3/2}(z), \tag{2}$$

where P = pressure, T = absolute temperature, v = specific volume, k = Boltzmann's constant, and

$$\lambda^2=2\pi\hbar^2/mkT. \tag{3}$$

The functions $f_{5/2}$ and $f_{3/2}$ are given by

$$f_{5/2}(z)=4\pi^{-1/2}\int_0^\infty dx\, x^2\ln(1+z\,e^{-x^2}), \tag{4}$$

$$f_{3/2}(z)=z(\partial/\partial z)f_{5/2}(z) = 4z\pi^{-1/2}\int_0^\infty dx\, x^2/(e^{x^2}+z). \tag{5}$$

Our goal is to solve (2) for z as a function of v/λ^3. As a first step, we define the function $D(\xi)$

$$D(\xi) = 1 - \frac{-4v}{\pi^{1/2}\lambda^3}\,\xi \int_0^\infty \frac{dx\; x^2}{\exp(x^2)+\xi}$$

$$= 1 - \frac{2v}{\pi^{1/2}\lambda^3}\,\xi \int_0^\infty \frac{dy\;(\ln\xi)^{1/2}}{y(y+\xi)}, \tag{6}$$

which is seen to be analytic in the ξ-plane cut on the real axis from -1 to $-\infty$. For large ξ, $D(\xi)$ has the expansion[2]

$$D(\xi) = \frac{4v}{3\pi^{1/2}\lambda^3}(\ln\xi)^{3/2} + 1 + O[(\ln\xi)^{-1/2}]. \tag{7}$$

For real positive v/λ^3, $D(\xi)$ has a single zero $\xi = z$ in the cut plane. This may be verified by simple means. We will use, however, the principle of the argument[3] which states that the number of zeros minus the number of poles of a function meromorphic within a contour C is $1/2\pi$ times the change in the argument of the function around C. Some of the notions involved will become useful later. For the function $D(\xi)$, we consider three parts of the closed contour as shown in Fig. 1. Because of its logarithmic behavior for large z, we have that $\arg D$ is constant for ξ on C_∞. Thus no change in the argument of D is experienced as ξ goes around C_∞. On $C_\pm$, the Plemelj formulas[4] give

$$D^\pm(\nu) = 1 - \frac{2v}{\pi^{1/2}\lambda^3}\,\nu \int_1^\infty \frac{dy(\ln y)^{1/2}}{y(y+\nu)}$$

$$\mp i2\pi^{1/2}(v/\lambda^3)[\ln(-\nu)]^{1/2},\ \nu \in C_\pm, \tag{8}$$

where the principal value of the integral is to be taken above. Since the real part of $D^\pm(\nu)$ increases monotonically from $-\infty$ to a positive constant ($\cong 1 + 2.612v/\lambda^3$) as ν goes from $-\infty$ to -1 and is of order $[\ln(-\nu)]^{3/2}$ for large negative ν, we see that the argument of $D(\xi)$ increases by π as ξ traverses C_+ and increases by another π as C_- is traversed. Hence $D(\xi)$ has one zero in the cut plane.

Consider now an analytic function $F(\xi)$ related to $D(\xi)$ as follows:

$$F(\xi)(z-\xi) = D(\xi). \tag{9}$$

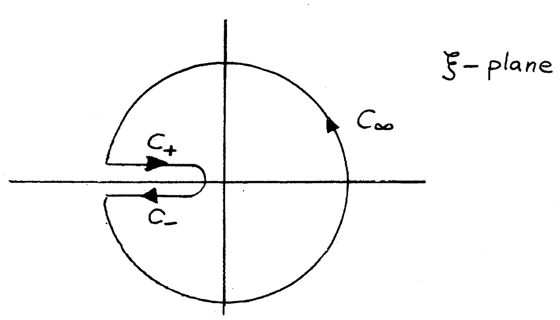

FIG. 1. The three parts of the closed contour of $D(\xi)$.

Thus F must be analytic in the plane cut from $-\infty$ to -1 and have no zeros or poles in the finite plane. We will now construct $F(\xi)$. We note that $D(\xi)/F(\xi)$ must be continuous across the cut, i.e.,

$$D^+(\nu)/F^+(\nu) - D^-(\nu)/F^-(\nu) = 0, \tag{10}$$

or

$$\frac{F^+(\nu)}{F^-(\nu)} = \frac{D^+(\nu)}{D^-(\nu)} = e^{2i\theta(\nu)}, \quad -\infty \leqslant \nu \leqslant -1, \tag{11}$$

where from Eq. (8) we see that θ is given by

$$\theta(\nu) = \tan^{-1}\left[\frac{2\pi^{1/2}(v/\lambda^3)[\ln(-\nu)]^{1/2}}{\dfrac{2}{\pi^{1/2}\lambda^3}\dfrac{v}{}\nu\displaystyle\int_1^\infty \frac{dy\;(\ln y)^{1/2}}{y(y+\nu)} - 1}\right]. \tag{12}$$

We take the branch of the $\tan^{-1}$ so that

$$\theta(-\infty) \equiv 0\ . \tag{13}$$

Equation (11) along with condition that F have no zeros or poles and have finite degree at infinity is known as the homogeneous Hilbert problem for $F(\xi)$.[4] The solution is obtained by noting that if we define

$$\Gamma(\xi) = (\xi/\pi)\int_{-\infty}^{-1}[\theta t\,\theta(t)/t(t-\xi)]\ , \tag{14}$$

then the limits of $\Gamma(\xi)$ on $C_\pm$ are given by

$$\Gamma^\pm(\nu) = (\nu/\pi)\int_{-\infty}^{-1}[dt\,\theta(t)/t(t-\nu)] \pm i\theta(\nu)\ , \tag{15}$$

and hence the function $\exp(\Gamma(\xi))$ satisfies the ratio condition [Eq. (11)]. But since $\theta(-1) = \pi$, we see from the calculation

$$\Gamma(\xi) = \frac{\xi}{\pi}\int_{-\infty}^{-1}\frac{[\theta(t)-\pi]dt}{t(t-\xi)} + \xi\int_{-\infty}^{-1}\frac{dt}{t(t-\xi)}$$

$$= \frac{\xi}{\pi}\int_{-\infty}^{-1}\frac{[\theta(t)-\pi]}{t(t-\xi)}\,dt + \ln(-1-\xi), \tag{16}$$

that $\exp(\Gamma(\xi))$ has a zero at $\xi = -1$. There are no other zeros or poles. Therefore

$$F(\xi) = [C/(1+\xi)]\exp(\Gamma(\xi)), \tag{17}$$

is the required solution determined up to the constant C. To find C and z we equate both sides of Eq. (9) and their derivatives at $\xi = 0$. The result for C is

$$C = v/\lambda^3 - [1 - (1/\pi)\int_{-\infty}^{-1} dt\,\theta(t)/t^2], \tag{18}$$

and finally the fugacity is given by

$$z = \{v/\lambda^3 - [1 - (1/\pi)\int_{-\infty}^{-1} dt\,\theta(t)/t^2]\}^{-1}, \tag{19}$$

with $\theta(t)$ given in Eq. (12).

IDEAL BOSE GAS

For a Bose gas of finite volume V, the fugacity-density equation is given by

$$\frac{1}{v}=\frac{1}{\lambda^3}\frac{4z}{\lambda^{1/2}}\int_0^\infty \frac{dx\, x^2}{\exp(x^2)-z}+\frac{1}{V}\frac{z}{1-z}. \qquad (20)$$

We consider then the function

$$E(\xi)=1-\frac{2v}{\pi^{1/2}\lambda^3}\xi\int_0^\infty \frac{dy\,(\ln y)^{1/2}}{y(y-\xi)}-\frac{1}{N}\frac{\xi}{1-\xi}, \qquad (21)$$

which has a single zero $\xi=z$ and a simple pole at $\xi=1$. The factor N is the number of particles. $E(\xi)$ also has a branch cut on the real axis from $+1$ to $+\infty$. The limiting values of $E(\xi)$ on the cut are

$$E^{\pm}(\nu)=1-\frac{2v}{\pi^{1/2}\lambda^3}\nu\int_1^\infty \frac{dy\,(\ln y)^{1/2}}{y(y-\nu)}$$

$$-(1/N)\,[\nu/(1-\nu)]\mp i2\pi^{1/2}(v/\lambda^3)(\ln\nu)^{1/2}, \qquad (22)$$

where $+(-)$ denotes the limit from above (below). We introduce a new function $B(\xi)$ given by

$$E(\xi)=B(\xi)[(z-\xi)/(\xi-1)], \qquad (23)$$

which has the same cut as does E but has no poles or zeros. Again we solve the Hilbert problem resulting from the fact that $E(\xi)/B(\xi)$ must be continuous across the cut. The result is

$$B(\xi)=K\exp[(\xi/\pi)\textstyle\int_1^\infty dt\,\varphi(t)/t(t-\xi)], \qquad (24)$$

where

$$\varphi(t)=\tan^{-1}\left[\frac{2\pi^{1/2}(v/\lambda^3)(\ln t)^{1/2}}{\frac{2vt}{\pi^{1/2}\lambda^3}\int_1^\infty \frac{dy\,(\ln y)^{1/2}}{y(y-t)}-\frac{1}{N}\frac{t}{t-1}-1}\right],$$

$$\varphi(0)=0. \qquad (25)$$

Finally, using Eq. (21) and its derivative at $\xi=0$, we find

$$z=\left(\frac{v}{\lambda^3}+1+\frac{1}{N}+\frac{1}{\pi}\int_1^\infty \frac{\varphi(t)dt}{t^2}\right)^{-1} \qquad (26)$$

$$K=-z^{-1} \qquad (27)$$

Equations (19) and (26), respectively, give the fugacity for the ideal Fermi gas as a function of v/λ^3 and the fugacity for the ideal Bose gas as a function of v/λ^3 and N. They are not particularly useful formulas, however, for extracting information in limiting cases ($v/\lambda^3 \gg 1$, etc.) and are therefore complementary to the known expansions[5] for these cases.

However, Eq. (23), for example, holds for any ξ. Therefore considerable freedom exists in developing other formulas for z. For instance, consider the limit as $\xi\to 1$ of Eq. (23) multiplied by $(\xi-1)$. We have

$$\frac{1}{N}=K(z-1)\exp\left(\frac{1}{\pi}\int_1^\infty \frac{\varphi(t)dt}{t(t-1)}\right). \qquad (28)$$

Using (27) we obtain

$$\frac{1}{z}=1+\frac{1}{N}\exp\left(-\frac{1}{\pi}\int_1^\infty \frac{\varphi(t)dt}{t(t-1)}\right). \qquad (29)$$

For $t\approx 1$, $\varphi(t)$ is approximately

$$\varphi(t)\approx\tan^{-1}\left[\frac{2\pi^{1/2}(v/\lambda^3)(t-1)^{1/2}}{(\frac{T}{T_c})^{3/2}-\frac{1}{N}\frac{1}{t-1}-1}\right] \qquad (30)$$

where $T_c=(2\pi\hbar^2/mk)(2.612v)^{-2/3}$. (31)

We consider three cases:

(i) $T>T_c$.

Here $\varphi(t)\approx-\pi$ for

$$t-1\gtrsim\{N[(T/T_c)^{3/2}-1]\}^{-1},$$

so that the integral in (29) blows up logarithmically as $N\to\infty$. We find that

$$z^{-1}=1+C_1[(T/T_c)^{3/2}-1]. \qquad (32)$$

(ii) $T<T_c$.

Now $\varphi(t)\approx-\pi/2$ for

$$2\pi^{1/2}(v/\lambda^3)(t-1)^{1/2}\gtrsim 1-(T/T_c)^{3/2}.$$

Therefore

$$Z^{-1}=1+C_2/\{N[1-(T/T_c)^{3/2}]\}.$$

(iii) $|1-(T/T_c)^{3/2}|\ll N^{-1/3}$.

For this final case we note that $\varphi(t)\approx-\pi/2$ for

$$2\pi^{1/2}\frac{v}{\lambda^3}(t-1)^{1/2}\gtrsim 1-(\frac{T}{T_c})^{3/2}+\frac{1}{N(t-1)} \qquad (33)$$

or

$$(t-1)^{1/2}\gtrsim 1-(\frac{T}{T_c})^{3/2}+N^{-1/3}\left(\frac{2\pi^{1/2}}{2.612}\right)^{2/3},$$

and thus

$$z=1+\frac{C_3}{N[1-(T/T_c)^{3/2}]+(2\pi^{1/2}N/2.612)^{2/3}}. \qquad (34)$$

The constants C_1, C_2, and C_3 above stay finite and positive as $N\to\infty$.

As a final note it should be pointed out that the pressure-fugacity relation may be inverted by the same procedure. For example, integration by parts in Eq. (4) gives for Eq. (1)

$$P\lambda^3/kT=(8z/3\pi^{1/2})\textstyle\int_0^\infty dx\,x^4/(e^{x^2}+z),$$

which is seen to be similar in form to the fugacity-density relation.

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[2]Ref. 1, p. 226.

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A Parametric Approach to the Ground-State Energy of an Electron Gas

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A parametric form is chosen for the ground-state wave function of an electron gas. The expression for the energy of the system is derived and then minimized with respect to the unknown parameters. The energies thus obtained agree well with the results of other authors.

I. INTRODUCTION

The problem of obtaining the ground-state energy of a quantum electron gas has been approached in a number of ways. The original work on this subject was done by Wigner,[1] who calculated the "correlation energy" of an electron gas for very high densities ($r_s < 1$) and then extended the results in such a way as to obtain the correct value at very low densities ($r_s >> 1$). He estimated his results to be correct everywhere to within 20%. Later calculations employing perturbation-expansion techniques[2-5] gave improved results for high densities while improved calculations for low densities[6] were carried out using Wigner's lattice model. In addition to Wigner's treatment, the region of metallic densities ($1 \lesssim r_s \lesssim 5$) has been treated[7] by truncating the Martin-Schwinger equations and using a random-phase approximation.[5] Finally, a recent paper[8] has shown how the problem may be treated by approximating the Slater sum for the system by an effective Boltzmann factor. The aim of this paper is to improve upon these calculations for the metallic density region, and also, to find a method which will give good agreement with the above-mentioned results in their respective regio gions of validity. It is further desirable that the method used for the electron gas be of sufficient flexibility so that it may later be generalized to include multicomponent systems. In accordance with these ideas, we shall present a parametric Rayleigh-Ritz variational method for calculating the ground-state energy, using a trial wave function of the form

$$\psi = D \exp\left(-\tfrac{1}{2}\sum_{i<j} u(r_{ij})\right), \qquad (1.1)$$

where $u(r)$ is an unknown function to be determined by variation and D is the wave function for an ideal gas of spin-$\frac{1}{2}$ particles.

II. DERIVATION OF THE BASIC EQUATION

The Hamiltonian operator H for an electron gas can be written as

$$H = -(\hbar^2/2m)\Delta^2 + V(\vec{r}_1 \cdots \vec{r}_N) , \qquad (2.1)$$

where $$\Delta^2 = \sum_{a=1}^{N} \nabla_a^2 \qquad (2.2)$$

and $V(\vec{r}_1 \cdots \vec{r}_N)$ represents the Coulomb potential. The expectation value of the energy $\langle E \rangle$, is then

$$\langle E \rangle = Q^{-1} \int \psi^* [-(\hbar^2/2m)\Delta^2 + V] \psi d\tau , \qquad (2.3)$$

where $$Q = \int \psi^* \psi d\tau , \qquad (2.4)$$

and $$d\tau \equiv d\vec{r}_1 d\vec{r}_2 \cdots d\vec{r}_N . \qquad (2.5)$$

We must now reduce this expression to a more tractable form in order to apply the variational principle.

First, we will treat the potential-energy term given by

$$\langle PE \rangle = Q^{-1} \int \psi^* V \psi d\tau . \qquad (2.6)$$

Since $V(\vec{r}_1 \cdots \vec{r}_n)$ represents the Coulomb potential, we may define a two-body term $v(r_{ij})$ in the following manner:

$$V(\vec{r}_1 \cdots \vec{r}_n) = \sum_{i<j} v(r_{ij}). \qquad (2.7)$$