UM-P-78/59

Ground-State Pressure of an Ideal Fermi Gas

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Abstract

A simple relationship between the pressure, internal energy and Fermi energy of an ideal ultra-degenerate Fermi gas is derived in two ways. The conditions for its validity and its use in simplifying calculations are discussed.

Introduction

The statistical mechanics of an ideal Fermi gas at zero temperature has been exhaustively studied. However, it appears that there is yet one more useful result which can be obtained for this system. This new result involves a relationship between the pressure, the internal energy and the Fermi energy of the gas. We have not seen it in any of the standard textbooks on statistical mechanics and thermodynamics, such as the modern ones by Huang[1], ter Haar[2] and Rief[3], or older ones by Tolman[4], Mayer and Mayer[5] and Guggenheim[6], although it is such a simple equation that it might exist somewhere in the ancient literature. We feel that it is useful firstly from a physical point of view, where its derivation will give some insight into handling the statistical mechanics involved with isotropic and anisotropic energy spectra, and secondly in detailed calculations where it is a considerable aid, as we shall see below.

Derivation

We begin by employing the thermodynamic relation for the pressure at zero temperature:

$$P = -\left(\frac{\partial U}{\partial V}\right)_S \tag{1}$$

where U is the internal energy of the gas, S is the entropy, and V is the volume of the system. Now by definition,

$$U = \sum_{\underset{\sim}{p},s} \varepsilon(\underset{\sim}{p},s)\ F(\underset{\sim}{p},s) \tag{2}$$

where $s = \pm 1$ is the spin quantum number, $\varepsilon(\underset{\sim}{p},s)$ is the energy of the fermion as a function of s and its momentum $\underset{\sim}{p}$, and $F(\underset{\sim}{p},s)$ is the Fermi-Dirac distribution function. In the thermodynamic limit, where $N \to \infty$, $V \to \infty$, but N/V is constant, we may take the sum over $\underset{\sim}{p}$ to an integral according to the prescription

$$\sum_{\underset{\sim}{p}} \to \frac{V}{h^3} \int d\underset{\sim}{p}$$

Now at zero temperature, we have

$$F(\underset{\sim}{p},s) = \begin{cases} 1 & \text{if} \quad \varepsilon(\underset{\sim}{p},s) \leq \varepsilon_F \\ 0 & \text{if} \quad \varepsilon(\underset{\sim}{p},s) > \varepsilon_F \end{cases}$$

where ε_F is the Fermi energy of the system. Equation (2) can then be written as

$$U = \frac{V}{h^3} \int d\underset{\sim}{p}\ \varepsilon(\underset{\sim}{p},s)\ \theta(\varepsilon_F - \varepsilon(\underset{\sim}{p},s)) \tag{3}$$

where θ is the Heaviside function. The Fermi energy is itself a function of the volume, since it is obtained from the number equation as follows:

$$N = \sum_{\underset{\sim}{p},s} F(\underset{\sim}{p},s) = \frac{V}{h^3} \sum_s \int d\underset{\sim}{p}\ \theta(\varepsilon_F - \varepsilon(\underset{\sim}{p},s)) \tag{4}$$

Differentiating Eq. (3) with respect to V, we obtain

$$\frac{\partial U}{\partial V} = \frac{U}{V} + \frac{V}{h^3} \sum_s \int d\underset{\sim}{p}\ \varepsilon(\underset{\sim}{p},s)\ \frac{\partial}{\partial V}\ \theta(\varepsilon_F - \varepsilon(\underset{\sim}{p},s))$$

or

$$\frac{\partial U}{\partial V} = \frac{U}{V} + \frac{V}{h^3} \frac{\partial \varepsilon_F}{\partial V} \sum_s \int d\underset{\sim}{p}\ \varepsilon(\underset{\sim}{p},s)\ \delta(\varepsilon_F - \varepsilon(\underset{\sim}{p},s)) \tag{5}$$

by definition of the Heaviside and δ-function. To obtain an expression for $\partial\varepsilon_F/\partial V$, we differentiate Eq. (4) with respect to V:

$$0 = \frac{N}{V} + \frac{V}{h^3} \frac{\partial \varepsilon_F}{\partial V} \sum_s \int d\underset{\sim}{p}\ \delta(\varepsilon_F - \varepsilon(\underset{\sim}{p},s)) \tag{6}$$

Eliminating $\partial\varepsilon_F/\partial V$ from Eqs. (5) and (6) and using Eq. (1), we obtain

$$P = -\frac{U}{V} + \frac{N}{V} \frac{G_1(\varepsilon_F)}{G_2(\varepsilon_F)} \tag{7}$$

where

$$G_1(\varepsilon_F) = \sum_s \int d\underset{\sim}{p}\ \varepsilon(\underset{\sim}{p},s)\delta(\varepsilon_F - \varepsilon(\underset{\sim}{p},s))$$

$$= \sum_s \iiint_{-\infty}^{\infty} dp_x\ dp_y\ dp_z\ \varepsilon(p_x,p_y,p_z,s)\delta(\varepsilon_F - \varepsilon(p_x,p_y,p_z,s))$$

and similarly

$$G_2(\varepsilon_F) = \sum_s \iiint_{-\infty}^{\infty} dp_x\ dp_y\ dp_z\ \delta(\varepsilon_F - \varepsilon(p_x,p_y,p_z,s)).$$

../3

Let us first perform the p_x-integral in G_1. Let $t = \varepsilon(p_x, p_y, p_z s)$, which can be inverted to obtain $p_x = f(t, p_y, p_z, s)$. Then $dp_x = (\partial f/\partial t)dt$, and

$$G_1(\varepsilon_F) = \sum_{s} \iint_{-\infty}^{\infty} dp_y \, dp_z \int_{\varepsilon(-\infty,p_y,p_z,s)}^{\varepsilon(\infty,p_y,p_z,s)} t \, \frac{\partial f}{\partial t} \, \delta(\varepsilon_F - t) dt .$$

Then

$$G_1(\varepsilon_F) = \varepsilon_F \sum_{s} \iint dp_y \, dp_z \left| \frac{\partial f(t,p_y,p_z,s)}{\partial t} \right|_{t = \varepsilon_F}$$

provided that $\varepsilon(-\infty,p_y,p_z,s) \leq \varepsilon_F \leq \varepsilon(\infty,p_y,p_z,s)$. This condition now furnishes the limits on p_y and p_z. It is easy to see that by making the same substitution in G_2 as for G_1, we have

$$G_1(\varepsilon_F) = \varepsilon_F \, G_2(\varepsilon_F). \tag{8}$$

Hence, from Eqs. (7) and (8), we finally obtain

$$P = -\frac{U}{V} + \frac{N\varepsilon_F}{V} . \tag{9}$$

The right-hand side of Eq. (9) is positive as required, since ε_F is the highest filled energy level, which implies $U < N\varepsilon_F$.

Some Simple Examples

We may check Eq. (9) by taking two simple cases. For the non-relativistic Fermi gas, where $\varepsilon(\underset{\sim}{p},s) = p^2/2m$, we have[1] $U = \frac{3}{5} N\varepsilon_F$, from which we immediately obtain $P = \frac{2}{5} N\varepsilon_F/V$, or $P = \frac{2}{3} U/V$. Again, for the ultra-relativistic Fermi gas, where $\varepsilon(\underset{\sim}{p},s) = pc$, we have[1] $U = \frac{3}{4} N\varepsilon_F$, and so from Eq. (9) we obtain $P = \frac{1}{4} N\varepsilon_F/V$ or $P = \frac{1}{3} U/V$.

Another (Kinetic) Derivation

Eq. (9) can be derived in another way. This derivation was motivated by our work on the equation of state of ideal relativistic neutrons in a magnetic field at zero temperature[7]. The energy levels of these neutrons are given by[8]

$$\varepsilon(p,s) = \left[p^2c^2 + \mu^2B^2 + m^2c^4 + 2\mu Bs(p^2c^2\sin^2\theta + m^2c^4)^{\frac{1}{2}}\right]^{\frac{1}{2}} \tag{10}$$

where μ is the magnetic moment of the neutron, $s = \pm 1$ is the spin quantum number, and θ is the angle between the momentum $\underset{\sim}{p}$ and the magnetic field B, which is taken to be in the z-direction. Since the energy of the particle is now anisotropic, the question of whether the pressure is also anistropic arises. To check this, we calculate the pressure elements of the stress-energy tension, P_{xx}, P_{yy}, P_{zz}, where

$$P_{xx} = \frac{1}{h^3} \sum_{s} \iiint_{-\infty}^{\infty} dp_x \, dp_y \, dp_z \, p_x \frac{\partial \varepsilon(\underset{\sim}{p},s)}{\partial p_x} \, \theta(\varepsilon_F - \varepsilon(\underset{\sim}{p},s)) \qquad (11)$$

where p_x is the x-component of the momentum, and as before the θ-function is just the Fermi-Dirac distribution function as zero temperature. P_{yy} and P_{zz} are defined similarly. The θ-function furnishes the limits on the p_x, p_y and p_z integrals: for example, to obtain the limits on p_x, we solve $\varepsilon_F = \varepsilon(p,s)$ for p_x, and obtain solutions $p_{x_1}(\varepsilon_F,p_y,p_z,s)$ and $p_{x_2}(\varepsilon_F,p_y,p_z,s)$, such that for $p_{x_1} \le p_x \le p_{x_2}$ we have $\varepsilon(\underset{\sim}{p},s) < \varepsilon_F$. Limits on the p_y and p_z integrals are obtained from similar considerations, so we now write

$$P_{xx} = \frac{1}{h^3} \sum_{s} \int_{P_{z_1}(\varepsilon_F,s)}^{P_{z_2}(\varepsilon_F,s)} dp_z \int_{P_{y_1}(\varepsilon_F,P_z,s)}^{P_{y_2}(\varepsilon_F,P_z,s)} dp_y \int_{P_{x_1}(\varepsilon_F,P_y,P_z,s)}^{P_{x_2}(\varepsilon_F,P_y,P_z,s)} dp_x \, p_x \frac{\partial \varepsilon(\underset{\sim}{p},s)}{\partial p_x} \qquad (12)$$

Doing the p_x-integral by parts gives

$$\int_{P_{x_1}}^{P_{x_2}} p_x \frac{\partial \varepsilon}{\partial p_x} dp_x = \Big[p_x \varepsilon(\underset{\sim}{p},s)\Big]_{P_{x_1}}^{P_{x_2}} - \int_{P_{x_1}}^{P_{x_2}} \varepsilon(\underset{\sim}{p},s) dp_x .$$

But by definition of p_{x_1} and p_{x_2}, we have

$$\varepsilon(p_{x_1},p_y,p_z,s) = \varepsilon(p_{x_2},p_y,p_z,s) = \varepsilon_F .$$

Hence, we may write Eq. (12) as

$$P_{xx} = -\frac{1}{h^3}\sum_s \int_{P_{z_1}}^{P_{z_2}} \int_{P_{y_1}}^{P_{y_2}} \int_{P_{x_1}}^{P_{x_2}} dp_x dp_y dp_z \, \varepsilon(\underset{\sim}{p},s)$$

$$+ \frac{\varepsilon_F}{h^3}\sum_s \int_{P_{x_1}}^{P_{z_2}} dp_z \int_{P_{y_1}}^{P_{y_2}} dp_y \, (p_{x_2} - p_{x_1})$$

$$= -\frac{U}{V} + \frac{\varepsilon_F}{h^3}\sum_s \int_{P_{z_1}}^{P_{z_2}} dp_z \int_{P_{y_1}}^{P_{y_2}} dp_y \int_{P_{x_1}}^{P_{x_2}} dp_x .$$

Hence

$$P_{xx} = -\frac{U}{V} + \frac{N\varepsilon_F}{V} \tag{13}$$

by Eq. (4). The same result may be obtained for P_{yy} by doing the integrations in the order $dp_z dp_x dp_y$, and similarly for P_{zz}.

Remarks and Conclusions

Since, as shown in Eq. (13), $P_{xx} = P_{yy} = P_{zz} = -\frac{U}{V} + \frac{N\varepsilon_F}{V}$, the pressure is isotropic and is given again by Eq. (9). This result is of course, only true if we can change the order of integrations, which is easy to verify, and if the allowed values of the particles' momenta are continuous. This second condition is essential for the result to hold. It is also necessary that the energy spectrum be a function only of the modulus of each momentum component, which will be true for all physically reasonable systems. In contrast, consider a gas of electrons in a magnetic field in the z-direction; the energy levels are given by the Dirac equation as[9]

$$\varepsilon(P_z,n,s) = [P_z{}^2c^2 + m^2c^4 + ehcB(2n - s + 1)]^{\frac{1}{2}} \tag{14}$$

where n = 0,1,2,..... This is the general Landau level spectrum which of course, includes the well-known non-relativistic results. The detailed statistical mechanics of this system has been studied by Chiu and Canuto[10]. Their results for the pressure establish that $P_{xx} = P_{yy} \neq P_{zz}$. We see that for this spectrum, Eq. (14), the momentum components in the x and y directions have been quantized into the appropriate Landau levels, and so the second condition mentioned above is not satisfied. For the spectrum given in Eq. (10), however, the allowed values of the momenta of the neutron are continuous, and thus $P_{xx} = P_{yy} = P_{zz}$ and now we have Eq. (9) holding.

We have tried to obtain a relationship between the pressure as given by Eq. (1) and any linear combination of the components P_{xx}, P_{yy} and P_{zz} for the system with the single-particle energy spectrum given by Eq. (14), using the detailed results given in ref. 10. We have not been able to find any general relationship of this kind for this system (where the spectrum is both anistropic and not a continuous function of all the momentum components). Thus we reiterate that only for the systems where the single particle energy spectrum is either isotropic in the momenta (for example $\varepsilon(\underset{\sim}{p}) = |\underset{\sim}{p}|^2/2m$ or $\varepsilon(\underset{\sim}{p}) = |\underset{\sim}{p}|c$) or anistropic in the momenta but a continuous function of all momentum components, as in Eq. (10), does $P_{xx} = P_{yy} = P_{zz} = P$ as given by Eq. (9) or Eq. (13).

For the simple examples we have given, using Eq. (9) is not much easier than differentiating the internal energy directly. However, in more complicated cases our result will simplify calculations considerably, since it avoids a possibly complicated differentiation of the internal energy with respect to the Fermi energy, and a further differentiation of the Fermi energy with respect to volume. For the system whose energy spectrum is given by Eq. (10), it is expecially useful, since in general the internal energy and the Fermi energy must be calculated numerically. We have discussed the thermodynamic properties of the system with this spectrum elsewhere[7], and have found that Eq. (9) has been most useful in the calculation of the pressure. In particular, in the ultra-high-field limit it readily yields $P = \frac{1}{2}\, U/V$.

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