

Electrical and Thermal Currents in a Slightly Ionized Gas*

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In this communication, the author has solved the Boltzmann equation for electrons in a slightly ionized gas under the influence of an electric field (ac+dc), a magnetic field and temperature gradient. Expressions for the electrical and thermal currents have been obtained in terms of integrals having collision frequency and f_0 , the isotropic part of the distribution function, in the integrand. A differential equation for f_0 has been set up and analytical expressions obtained under simplifying assumptions. The application of the analysis to transport properties and electromagnetic wave propagation has also been indicated.

INTRODUCTION

IN this communication, the author has investigated the electrical and thermal currents in a slightly ionized uniform gas, under the influence of temperature gradients, a magnetic field, a stationary electric field, and an alternating electric field. Many investigations¹ in this area have been published but none seems to be so general. Usually the investigators have neglected temperature gradients, assumed the magnetic field to be perpendicular to the electric field and considered only one type (ac or dc) of electric field. Some investigators have assumed a constant collision frequency independent of electron velocity, which severely limits the applicability of their results.

The author has solved the Boltzmann equation and obtained expressions for the three components of electrical and thermal currents involving integrals having collision frequency and f_0 , the isotropic part of distribution function. Assuming the collisions between electrons and neutral molecules to be elastic, a differential equation for f_0 involving a collision frequency, temperature gradient, electric field, and magnetic field has been set up. Analytical solutions for some special cases have been obtained.

The application of this analysis to the study of the propagation of an electromagnetic wave in the gas and transport properties of the gas has also been discussed.

BOLTZMANN'S EQUATION

Boltzmann's transfer equation may be written as

$$\frac{\partial f}{\partial t} + \alpha_x \frac{\partial f}{\partial v_x} + \alpha_y \frac{\partial f}{\partial v_y} + \alpha_z \frac{\partial f}{\partial v_z} + v_x \frac{\partial f}{\partial x} + v_y \frac{\partial f}{\partial y} + v_z \frac{\partial f}{\partial z} = \left(\frac{\partial f}{\partial t} \right)_c, \quad (1)$$

where $f(\mathbf{v})$ is the distribution function of electron velocities, t is the time, α is the acceleration of electrons, \mathbf{v} is the electron velocity, x, y, z are space coordinates,

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¹ W. P. Allis, *Handbuch der Physik*, edited by S. Flügge (Springer-Verlag, Berlin, 1956), pp. 21, 383; L. Mower, *Phys. Rev.* **116**, 16 (1959) (assessment of recent publications).

and $(\partial f / \partial t)_c$ is the rate of change of f due to collisions.

The acceleration α of electrons in the presence of an electric field $\mathbf{E}_0 + \mathbf{E} \exp(i\omega_0 t)$ and a magnetic field \mathbf{B} is given by

$$-\alpha = \mathbf{a} + \mathbf{A} \exp(i\omega_0 t) + \mathbf{v} \times \boldsymbol{\omega}, \quad (2)$$

where

$$\mathbf{a} = q\mathbf{E}_0/m,$$

$$\mathbf{A} = q\mathbf{E}/m,$$

$$\boldsymbol{\omega} = q\mathbf{B}/mc_0,$$

q is the electronic charge, m is the electronic mass, and c_0 is the velocity of light in vacuum.

The distribution function may be expressed as

$$f(\mathbf{v}) = f_0 + v_x \mu_x + v_y \mu_y + v_z \mu_z, \quad (3)$$

where

$$\mu_x = f_x + f'_x \exp(i\omega_0 t) = f_x + g_x \cos \omega_0 t + h_x \sin \omega_0 t, \quad (3A)$$

$$\mu_y = f_y + f'_y \exp(i\omega_0 t) = f_y + g_y \cos \omega_0 t + h_y \sin \omega_0 t, \quad (3B)$$

$$\mu_z = f_z + f'_z \exp(i\omega_0 t) = f_z + g_z \cos \omega_0 t + h_z \sin \omega_0 t, \quad (3C)$$

and $f_0, f_x, f_y, f_z, g_x, g_y, g_z, h_x, h_y, h_z, f'_x, f'_y$ and f'_z are functions of v only. From Eqs. (3A), (3B), and (3C) we have

$$f'_x = g_x - ih_x; \quad f'_y = g_y - ih_y; \quad f'_z = g_z - ih_z. \quad (4)$$

From Eq. (2) we obtain

$$\partial f / \partial v_x = v_x F_1(v) + \mu_x, \quad (5A)$$

$$\partial f / \partial t = \sum i\omega_0 v_x f'_x, \quad (5B)$$

where

$$F_1(v) = \frac{1}{v} \frac{\partial f_0}{\partial v} + \sum \left(\frac{v_x}{v} \frac{\partial \mu_x}{\partial v} \right).$$

Assuming constant electron density, we further obtain

$$\alpha_x \frac{\partial f}{\partial v_x} + v_x \frac{\partial f}{\partial x} = (\alpha_x - b_x v^2) \frac{\partial f}{\partial v_x} = -(\beta_x + v_y \omega_z - v_z \omega_y) \frac{\partial f}{\partial v_x}, \quad (6)$$

where

$$\beta_x = a_x + A_x \exp(i\omega_0 t) + b_x v^2,$$

and

$$b_x = (1/2T) \partial T / \partial x.$$

For a Lorentzian gas consisting of neutral molecules and electrons, a reasonable assumption for slightly ionized gases it may be shown² that

$$\left(\frac{\partial f}{\partial t}\right)_c = -\nu(f-f_0) + \frac{m}{Mv^2} \frac{\partial}{\partial v}(f_0 v^3 \nu) + \frac{kT}{Mv^2} \frac{\partial}{\partial v} \left(\nu v^2 \frac{\partial f_0}{\partial v} \right), \quad (7)$$

where ν is the collision frequency of electrons, M is the mass of molecules, k is the Boltzmann constant, and T the temperature of the gas.

Using Eqs. (2), (3), (5), and (7), putting $\langle v_x^2 \rangle_{av} = \langle v_y^2 \rangle_{av} = \langle v_z^2 \rangle_{av} = v^2/3$ and $\langle v_x v_y \rangle_{av} = \langle v_y v_z \rangle_{av} = \langle v_z v_x \rangle_{av} = 0$ and equating the terms having v_x , v_y , and v_z and the remaining terms on both sides of Eq. (1), we obtain

$$\frac{m}{M} \frac{\partial}{\partial v} (\nu f_0 v^3) + \frac{kT}{M} \frac{\partial}{\partial v} \left(\nu v^2 \frac{\partial f_0}{\partial v} \right) = -\frac{1}{3v^2} \sum \beta_x \frac{\partial}{\partial v} (\mu_x v^3), \quad (8)$$

$$\frac{\beta_x}{v} \frac{\partial f_0}{\partial v} + \omega_y \mu_x - \omega_z \mu_y - \frac{\partial \mu_x}{\partial t} = \nu \mu_x, \quad (9A)$$

$$\frac{\beta_y}{v} \frac{\partial f_0}{\partial v} + \omega_z \mu_x - \omega_x \mu_z - \frac{\partial \mu_y}{\partial t} = \nu \mu_y, \quad (9B)$$

$$\frac{\beta_z}{v} \frac{\partial f_0}{\partial v} + \omega_x \mu_y - \omega_y \mu_x - \frac{\partial \mu_z}{\partial t} = \nu \mu_z. \quad (9C)$$

Equating the time dependent and time independent terms on both sides of Eq. (9), we arrive at the following relations:

$$\frac{(a_x + b_x v^2)}{v} \frac{\partial f_0}{\partial v} + \omega_y f_z - \omega_z f_y = \nu f_x, \quad (10A)$$

$$\frac{(a_y + b_y v^2)}{v} \frac{\partial f_0}{\partial v} + \omega_z f_x - \omega_x f_z = \nu f_y, \quad (10B)$$

$$\frac{(a_z + b_z v^2)}{v} \frac{\partial f_0}{\partial v} + \omega_x f_y - \omega_y f_x = \nu f_z, \quad (10C)$$

$$\frac{A_x}{v} \frac{\partial f_0}{\partial v} + \omega_y f_z' - \omega_z f_y' = (\nu + i\omega_0) f_x', \quad (11A)$$

$$\frac{A_y}{v} \frac{\partial f_0}{\partial v} + \omega_z f_x' - \omega_x f_z' = (\nu + i\omega_0) f_y', \quad (11B)$$

$$\frac{A_z}{v} \frac{\partial f_0}{\partial v} + \omega_x f_y' - \omega_y f_x' = (\nu + i\omega_0) f_z'. \quad (11C)$$

² S. Chapman and T. G. Cowling, *Mathematical Theory of Nonuniform Gases* (Cambridge University Press, New York, 1939), p. 348; P. M. Morse, W. P. Allis, and E. S. Lamar, *Phys. Rev.* 48, 412 (1935).

Solving Eqs. (10A), (10B), and (10C) for f_x , f_y , and f_z we obtain

$$f_x = \frac{F_x}{v} \frac{\partial f_0}{\partial v} + \nu F_x' \frac{\partial f_0}{\partial v}, \quad (12A)$$

$$f_y = \frac{F_y}{v} \frac{\partial f_0}{\partial v} + \nu F_y' \frac{\partial f_0}{\partial v}, \quad (12B)$$

$$f_z = \frac{F_z}{v} \frac{\partial f_0}{\partial v} + \nu F_z' \frac{\partial f_0}{\partial v}, \quad (12C)$$

where

$$F_x = \frac{a_x(\nu^2 + \omega_x^2) + a_y(\omega_x \omega_y - \nu \omega_z) + a_z(\omega_z \omega_x + \nu \omega_y)}{\nu(\nu^2 + \omega^2)}, \quad (12D)$$

$$F_x' = \frac{b_x(\nu^2 + \omega_x^2) + b_y(\omega_x \omega_y - \nu \omega_z) + b_z(\omega_z \omega_x + \nu \omega_y)}{\nu(\nu^2 + \omega^2)}, \quad (12E)$$

$$F_y = \frac{a_y(\nu^2 + \omega_y^2) + a_x(\omega_y \omega_z - \nu \omega_x) + a_z(\omega_z \omega_y + \nu \omega_x)}{\nu(\nu^2 + \omega^2)}, \quad (12F)$$

$$F_y' = \frac{b_y(\nu^2 + \omega_y^2) + b_x(\omega_y \omega_z - \nu \omega_x) + b_z(\omega_z \omega_y + \nu \omega_x)}{\nu(\nu^2 + \omega^2)}, \quad (12G)$$

$$F_z = \frac{a_z(\nu^2 + \omega_z^2) + a_x(\omega_z \omega_x - \nu \omega_y) + a_y(\omega_z \omega_y + \nu \omega_x)}{\nu(\nu^2 + \omega^2)}, \quad (12H)$$

$$F_z' = \frac{b_z(\nu^2 + \omega_z^2) + b_x(\omega_z \omega_x - \nu \omega_y) + b_y(\omega_z \omega_y + \nu \omega_x)}{\nu(\nu^2 + \omega^2)}. \quad (12I)$$

Solving Eqs. (11A), (11B), and (11C) for f_x' , f_y' , and f_z' and using Eq. (4), we obtain

$$g_x = (1/v) (\partial f_0 / \partial v) G_x, \quad (13A)$$

$$g_y = (1/v) (\partial f_0 / \partial v) G_y, \quad (13B)$$

$$g_z = (1/v) (\partial f_0 / \partial v) G_z, \quad (13C)$$

$$h_x = (1/v) (\partial f_0 / \partial v) H_x, \quad (13D)$$

$$h_y = (1/v) (\partial f_0 / \partial v) H_y, \quad (13E)$$

$$h_z = (1/v) (\partial f_0 / \partial v) H_z, \quad (13F)$$

where

$$G_x = \{ \nu(\nu^2 - 3\omega_0^2 + \omega^2) [A_x(\nu^2 - \omega_0^2 + \omega_x^2) + A_y(\omega_x \omega_y - \nu \omega_z) + A_z(\omega_z \omega_x + \nu \omega_y)] + \omega_0^2(3\nu^2 - \omega_0^2 + \omega^2)(2A_x \nu - A_y \omega_z + A_z \omega_y) \} \times [(\nu^2 + \omega_0^2)(\nu^2 + \omega_0^2 + \omega^2 + 2\omega_0 \omega) \times (\nu^2 + \omega_0^2 + \omega^2 - 2\omega_0 \omega)]^{-1}, \quad (14A)$$

$$H_x = \omega_0 \{ (3\nu^2 - \omega_0^2 + \omega^2) [A_x(\nu^2 - \omega_0^2 + \omega_x^2) + A_y(\omega_x \omega_y - \nu \omega_z) + A_z(\omega_z \omega_x + \nu \omega_y)] - \nu(\nu^2 - 3\omega_0^2 + \omega^2)(2A_x \nu - A_y \omega_z + A_z \omega_y) \} \times [(\nu^2 + \omega_0^2)(\nu^2 + \omega_0^2 + \omega^2 + 2\omega_0 \omega) \times (\nu^2 + \omega_0^2 + \omega^2 - 2\omega_0 \omega)]^{-1}, \quad (14B)$$

and the expressions for G_y , H_y , G_z , and H_z are in symmetry with Eqs. (14A) and (14B).

ELECTRICAL AND THERMAL CURRENTS

The electrical and thermal currents, which are associated with an electron having velocity \mathbf{v} are given by

$$\mathbf{j} = -q\mathbf{v} \quad \text{and} \quad \mathbf{c} = (mv^2/2)\mathbf{v}.$$

Hence, using Eqs. (3), (12), and (13), the electrical and thermal currents due to electrons are given by

$$J_x = - \int \int \int q v_x f d\sigma_1 = - \int \int \int q v_x^2 \mu_x d\sigma_1 = (nq/3)(\Phi_x + \psi_x), \quad (15A)$$

$$J_y = - \int \int \int q v_y f d\sigma_1 = (nq/3)(\Phi_y + \psi_y), \quad (15B)$$

$$J_z = - \int \int \int q v_z f d\sigma_1 = (nq/3)(\Phi_z + \psi_z), \quad (15C)$$

$$C_x = + \int \int \int \frac{mv^2}{2} v_x f d\sigma_1 = + \int \int \int \frac{mv^2}{2} v_x^2 \mu_x d\sigma_1 = - \frac{nm}{6}(\Phi_x' + \psi_x'), \quad (15D)$$

$$C_y = \int \int \int \frac{mv^2}{2} v_y f d\sigma_1 = - \frac{nm}{6}(\Phi_y' + \psi_y'), \quad (15E)$$

$$C_z = \int \int \int \frac{mv^2}{2} v_z f d\sigma_1 = - \frac{nm}{6}(\Phi_z' + \psi_z') \quad (15F)$$

where

$$d\sigma_1 = dv_x dv_y dv_z,$$

$\langle v_x \rangle_{av} = \langle v_y \rangle_{av} = \langle v_z \rangle_{av} = \langle v_x v_y \rangle_{av} = \langle v_y v_z \rangle_{av} = \langle v_x v_z \rangle_{av} = 0$ by symmetry, v_x^2 , v_y^2 , and v_z^2 have been replaced by $v^2/3$, $d\sigma_1$ has been replaced by $4\pi v^2 dv$, the triple integrals have been replaced by single integrals extending from 0 to ∞ ,

$$\Phi_x = - \frac{4\pi}{n} \int_0^\infty (F_x + G_x \cos \omega_0 t + H_x \sin \omega_0 t) v^3 \frac{\partial f_0}{\partial v} dv, \quad (16A)$$

$$\psi_x = - \frac{4\pi}{n} \int_0^\infty F_x' v^5 \frac{\partial f_0}{\partial v} dv, \quad (16B)$$

$$\Phi_x' = - \frac{4\pi}{n} \int_0^\infty (F_x + G_x \cos \omega_0 t + H_x \sin \omega_0 t) v^5 \frac{\partial f_0}{\partial v} dv, \quad (16C)$$

$$\psi_x' = - \frac{4\pi}{n} \int_0^\infty F_x' v^7 \frac{\partial f_0}{\partial v} dv. \quad (16D)$$

Φ_y , Φ_y' , ψ_y , ψ_y' , Φ_z , Φ_z' , ψ_z , and ψ_z' are given by expressions symmetrical to Eqs. (16), and n is the electron density.

The following relations are helpful in evaluating the above integrals. If

$$\zeta(v) = - \frac{4\pi}{n} \int_0^\infty \xi(v) \frac{\partial f_0}{\partial v} dv,$$

then

$$\zeta = \left\langle \frac{1}{v^2} \frac{\partial \xi}{\partial v} \right\rangle \quad \text{if } \xi \neq \text{constant},$$

$$\zeta = - \frac{4\pi \xi}{n} [f_0]_0^\infty \quad \text{if } \xi = \text{constant},$$

$$\zeta = \frac{m}{kT} \left\langle \frac{\xi}{v} \right\rangle \quad \text{if } f_0 \propto \exp(-mv^2/2kT), \text{ i.e., Maxwellian.}$$

By using suitable auxiliary conditions expressions for well-known transport properties may be derived from Eqs. (15) and (16).

EVALUATION OF f_0

Using Eqs. (3), (8), (12), and (13), and averaging over one cycle we obtain

$$\begin{aligned} -\frac{1}{3} \sum (a_x + b_x v^2) \frac{\partial}{\partial v} \left\{ v^3 \left[\frac{F_x}{v} + v F_x' \right] \frac{\partial f_0}{\partial v} \right\} \\ - \frac{1}{6} \sum \frac{\partial}{\partial v} \left(\frac{A_x G_x}{v} \frac{\partial f_0}{\partial v} v^3 \right) \\ = - \frac{m}{M} \frac{\partial}{\partial v} (v f_0 v^3) + \frac{kT}{M} \frac{\partial}{\partial v} \left(v^2 \frac{\partial f_0}{\partial v} \right). \quad (17) \end{aligned}$$

This equation has in general to be solved numerically for f_0 with the boundary conditions $\partial f_0 / \partial v = 0$ and $f_0 = 1$ (arbitrary) at $v = 0$. The distribution function is $C_1 f_0$ where

$$C_1 \int_0^\infty 4\pi v^2 f_0 dv = n.$$

EVALUATION OF f_0 FOR ISOTHERMAL PLASMA

For an isothermal plasma $b_x = b_y = b_z = 0$ and Eq. (17) after simplification reduces to

$$\begin{aligned} - \frac{1}{3} \frac{\partial}{\partial v} \left\{ v^2 \nu S(v) \frac{\partial f_0}{\partial v} \right\} = \frac{m}{M} \frac{\partial}{\partial v} (v f_0 v^3) \\ + \frac{kT}{M} \frac{\partial}{\partial v} \left(v^2 \frac{\partial f_0}{\partial v} \right), \quad (18A) \end{aligned}$$

where

$$S(v) = \frac{a^2 v^2 + (a_x \omega_x + a_y \omega_y + a_z \omega_z)^2}{v^2 (v^2 + \omega^2)} + \frac{1}{2} \left(\frac{A^2 (v^2 + \omega_0^2) (v^2 + \omega_0^2 + \omega^2) + (v^2 - 3\omega_0^2 + \omega^2) (A_x \omega_x + A_y \omega_y + A_z \omega_z)^2}{(v^2 + \omega_0^2) (v^2 + \omega^2 + \omega_0^2 - 2\omega_0 \omega) (v^2 + \omega^2 + \omega_0^2 + 2\omega_0 \omega)} \right). \quad (18B)$$

Integrating Eq. (18) and putting $v=0$, we find the constant of integration to be zero. Further putting $\eta = (m/2kT)^{1/2}v$, we obtain

$$\frac{\partial f_0}{\partial \eta^2} \left(1 + \frac{M}{3kT} S(\eta) \right) + f_0 = 0. \quad (19)$$

The solution of Eq. (19) is

$$f_0 = C_1 \exp \left(- \int_0^{\eta^2} \frac{d\eta^2}{1 + (M/3kT)S(\eta)} \right). \quad (20)$$

Equation (20) may be expressed analytically in the following cases:

1. When the collision frequency is independent of electron velocity, $S(\eta)$ is constant and Eq. (20) yields

$$f_0 = C_1 \exp \left(\frac{-\eta^2}{1 + (M/3kT)S(\eta)} \right). \quad (20A)$$

This corresponds to a Maxwellian distribution with effective temperature T_e given by

$$T_e = T + (M/3k)S(\eta).$$

2. In the absence of magnetic field, $\omega_x = \omega_y = \omega_z = 0$, Eq. (18B) simplifies to

$$S(\eta) = \frac{a^2}{v^2} + \frac{A^2}{2(v^2 + \omega_0^2)},$$

which makes Eq. (20), integrable when $v = \eta/l$.

3. In the absence of alternating electric field, $A_x = A_y = A_z = A = 0$, and when the magnetic field is perpendicular to the electric field, Eq. (18B) reduces to

$$S(\eta) = a^2/(v^2 + \omega^2).$$

Substituting $v = \eta/l$ and the above equation in Eq. (20), we find the distribution function to be given by

$$f_0(\eta) = C_1 [\eta^2 + l^2(\omega^2 + MA^2/3kT)]^{p/2} \exp(-\eta^2). \quad (20B)$$

where $p = MA^2 l^2 / 3kT$.

4. In the absence of dc electric field and the magnetic field, Eq. (18B) reduces to

$$S(\eta) = A^2/2(v^2 + \omega_0^2).$$

Substituting $v = \eta/l$ and the above equation in Eq. (20) we obtain

$$f_0(\eta) = C_1 [\eta^2 + l^2(\omega_0^2 + MA^2/6kT)]^{p/2} \exp(-\eta^2), \quad (20C)$$

which has been obtained by Margenau.³

5. In the absence of dc magnetic field and when the

magnetic field is perpendicular to ac electric field

$$S(\eta) = \frac{A^2}{2} \frac{(v^2 + \omega_0^2 + \omega^2)}{(v^2 + \omega^2 + \omega_0^2)^2 - 4\omega_0^2 \omega^2},$$

which makes Eq. (20) integrable for $v = \eta/l$.

NONISOTHERMAL PLASMA—ZERO ELECTRIC FIELD

We consider the case when there is no electric field present, i.e., $a = A = 0$. Equation (17) simplifies to

$$-\frac{v^2}{3} \frac{\partial}{\partial v} \left(\nu v^3 S_1(v) \frac{\partial f_0}{\partial v} \right) = \frac{m}{M} \frac{\partial}{\partial v} (\nu f_0 v^3) + \frac{kT}{M} \left(\nu v^2 \frac{\partial f_0}{\partial v} \right), \quad (21)$$

where

$$S_1(v) = v \frac{b^2 v^2 + (b_x \omega_x + b_y \omega_y + b_z \omega_z)^2}{v^2(v^2 + \omega^2)}.$$

Putting $v = B/v^3$ as a special case in Eq. (21), we get

$$-\frac{v^2}{3} \frac{\partial}{\partial v} \left(S_1(v) \frac{\partial f_0}{\partial v} \right) = \frac{m}{M} \frac{\partial f_0}{\partial v} + \frac{kT}{M} \frac{\partial}{\partial v} \left(\frac{1}{v} \frac{\partial f_0}{\partial v} \right),$$

or

$$\left(\frac{kT}{Mv} + \frac{v^2 S_1}{3} \right) \frac{\partial^2 f_0}{\partial v^2} = \left(-\frac{m}{M} - \frac{v^2}{3} \frac{\partial S_1}{\partial v} + \frac{kT}{Mv^2} \right) \frac{\partial f_0}{\partial v},$$

or

$$f_0 = (\text{constant}) \int dv \exp \left\{ \int \left[\left(-\frac{m}{M} - \frac{v^2}{3} \frac{\partial S_1}{\partial v} + \frac{kT}{Mv^2} \right) / \left(\frac{kT}{Mv} + \frac{v^2 S_1}{3} \right) \right] dv \right\}. \quad (21A)$$

DISCUSSION

Propagation of an Electromagnetic Wave

The wave equation for a neutral gas in esu may be written as

$$\nabla^2 \mathbf{E} = \frac{1}{c^2} \frac{\partial^2 \mathbf{E}}{\partial t^2} + \frac{4\pi}{c^2} \frac{\partial \mathbf{J}}{\partial t}, \quad (22)$$

where \mathbf{E} is the electric vector. Combining Eq. (22) with Eqs. (15A), (15B), and (15C) giving \mathbf{J} in terms of \mathbf{E} , we arrive at partial differential equation in \mathbf{E} which may be solved.

It may be seen that the dc electric field and temperature gradient do not directly enter this problem but they affect the propagation through f_0 . The instantaneous power of electromagnetic wave dissipated per

³ H. Margenau, Phys. Rev. 69, 508 (1946).

unit volume is approximately given by

$$P = J_x E_x + J_y E_y + J_z E_z.$$

Transport Properties

Equations (15) expresses the thermal and electrical currents in terms of temperature gradient, electric

field and magnetic field. Expressions for transport properties may be found by using suitable sets of auxiliary conditions.

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Cluster Integrals and the Ground State of Bosons with Repulsive Interactions

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The properties of a Bose system of particles with repulsive interactions have previously been treated using perturbation theory in the formalism of second quantization. Others have also considered this problem by dealing with the wave function in configuration space, using the theory of cluster expansions. In these latter papers, variation with respect to a parameter in a trial function for the ground state has been shown to yield a ground-state energy close to the exact asymptotic expressions obtained from perturbation theory. The connection between the two methods is not immediately obvious from these cluster expansion treatments. It is shown here that, as one might expect, the cluster integral method can be handled so that it is completely equivalent to the pair approximation in perturbation theory.

1. INTRODUCTION

THE properties of a Bose system of particles with repulsive interactions has been treated using the formalism of second quantization by several investigators.¹⁻³ More recently^{4,5} the same problem has been considered dealing directly with the wave function in configuration space, using the theory of cluster expansions first introduced in statistical mechanics.⁶ In these latter treatments the ground-state wave function is expressed as a product of pair functions. The problem of evaluating the expectation value for the energy then becomes analogous to evaluating the classical partition function for an imperfect gas, expressed in terms of Mayer's cluster integrals. By considering only contributions to the energy from ring integrals, a tractable expression for the ground-state energy at low densities is obtained. Then a choice for the pair function is made and subsequent variation with respect to a parameter in this trial function has been shown to yield a ground-state energy quite close to the exact asymptotic expression obtained in references 2 and 3 above, where the contribution to the energy from pair excitations was calculated exactly.

Now one might naturally ask how this cluster integral method in configuration space is related to the pertur-

bation theory calculation using momentum-space eigenfunctions. An analogous situation exists for the calculation of the partition function of an ideal Bose gas, where there is a cluster integral development which is completely equivalent to the more usual sum-over-states.⁷ One might expect that here as well, the pair approximation perturbation theory should have its exact counterpart in a configuration space cluster integral development. Our purpose is to show that this expectation is indeed fulfilled. The cluster integral calculations previously made are not directly comparable to the perturbation theory calculations simply because the class of ring integrals which were taken as contributing to the ground-state energy do not correspond to the pair approximation of perturbation theory. The pair approximation yields a ground state which in configuration space has the form [see Eq. (A.21) of Appendix II of reference 3]

$$\Psi = \prod'_{i < j=1}^N [1 + f(r_{ij})], \quad (1)$$

where the prime denotes that in the expanded product for Ψ all terms with repeated particle indices are omitted. The prohibition of repeated indices is essential for the pair approximation, since the Fourier transform of a term with one repeated index, such as $f(r_{12})f(r_{23})$ shows that this term refers to excitation of three particles having momenta $\mathbf{k}_1, \mathbf{k}_2, \mathbf{k}_3$ with $\mathbf{k}_1 + \mathbf{k}_2 + \mathbf{k}_3 = 0$.³ The previous cluster integral developments do not

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³ T. D. Lee, K. Huang, and C. N. Yang, *Phys. Rev.* **106**, 1135 (1957).

⁴ F. Iwamoto, *Progr. Theoret. Phys. (Kyoto)* **19**, 597 (1958).

⁵ J. B. Aviles, *Ann. Phys.* **5**, 251 (1958).

⁶ J. E. Mayer and M. G. Mayer, *Statistical Mechanics* (John Wiley & Sons, Inc., New York, 1950), Chap. 13.

⁷ B. Kahn and G. E. Uhlenbeck, *Physica* **5**, 399 (1938).