ON THE STATISTICAL TREATMENT OF THE FERMION GAS I

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A new statistical method, very similar to the one generalized to contain the Weizsäcker inhomogenity correction modified by Gombás, is derived. With regard to the approximations introduced the summation over quantum states need not be approximated by integration but can be carried out exactly. In addition to the determination of the density from the variation principle more accurate methods are described. It is shown that from Plaskett's equation the density can only be determined within the classical ,,allowed zone" and the proper equation for the ,,forbidden zone" is given.

1. Introduction

For the interpretation of the bound state of systems consisting of particles with spin 1/2 the statistical method was first developed by THOMAS [1] and FERMI [2], who worked independently of each other. Later on the statistical method was improved in two main fields. On the one hand in order to calculate the energy due to the interaction of particles more accurately, the theory was generalized by DIRAC [3] to contain the exchange interaction and by GOMBÁS [4] to contain the correlation correction. These attempts, however, failed to eliminate the essential shortcomings of the density calculated on the basis of the Thomas-Fermi method. It is a common characteristic of all the investigations aiming at the correction of these defects that they are essentially independent of the interaction of the particles. In this connection I would like to refer to the papers of WEIZSÄCKER [5], GOMBÁS [6] and PLASKETT [7], which are the papers most closely related to the present one. It will be shown that the Weizsäcker inhomogeneity correction modified by GOMBÁS and the generalization of the Thomas-Fermi method suggested by PLASKETT can be traced back to a common basis further that the method described here can be regarded as an improved version of these methods.

In connection with the statistical energy expression obtained here it is suitable to make the following preliminary comment. In deriving the Thomas-Fermi statistical energy expression with the aid of the Wentzel-Kramers-Brillouin (WKB) method MARCH and PLASKETT [8] have shown that the statistical method involves two essential approximations as compared with the exact wave mechanical calculation. On the one hand it is based on the results

of the WKB method and on the other it approximates the summation over the quantum states by integration. To correct the latter error MARCH and PLASKETT apply the Euler-Maclaurin formula which makes a more accurate evaluation of the summation possible. In a former paper [9] we have shown that with a certain approximating assumption the summation over the quantum states can be carried out exactly. In the present paper this approximating assumption is necessarily involved thus the exact summation of the quantum states becomes possible.

We begin our investigation with wave mechanical considerations. Starting from the Schrödinger equation of n fermions we consider the form the one-particle state equations take if one-particle wave functions not orthogonal to each other are chosen. The equations thus obtained underlie the derivation of a new statistical model.

We now disregard the interaction of particles and restrict ourselves to the one-dimensional problem.

2. Non-orthogonal one-particle wave function system

The Schrödinger equation of n particles in the potential field $V(x)$ is

$$\sum_{i=1}^{n} H(x_i) \, \Phi = \mathscr{E} \, \Phi \,, \tag{1}$$

where

$$H(x) = -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + V(x) \tag{1'}$$

is the one-particle Hamiltonian.

Apart from the normalization constant a proper antisymmetrical solution of this equation is

$$\Phi = \begin{vmatrix} \varphi_1^0(x_1)\,\chi_-(\sigma_1) & \cdots & \varphi_1^0(x_n)\,\chi_+(\sigma_n) \\ \varphi_\pm^0(x_1)\,\chi_-(\sigma_1) & \cdots & \varphi_1^0(x_n)\,\chi_-(\sigma_n) \\ \cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots \\ \cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots \\ \varphi_f^0(x_1)\,\chi_+(\sigma_1) & \cdots & \varphi_f^0(x_n)\,\chi_-(\sigma_n) \\ \varphi_f^0(x_1)\,\chi_-(\sigma_1) & \cdots & \varphi_f^0(x_n)\,\chi_-(\sigma_n) \\ \varphi_g^0(x_1)\,\chi_\pm(\sigma_1) & \cdots & \varphi_g^0(x_n)\,\chi_\pm(\sigma_n) \end{vmatrix}, \tag{2}$$

if the one-particle wave functions satisfy the equation

$$H \varphi^0 (x) = \varphi^0 (x) E . \qquad (3)$$

Here $\varphi^0(x)$ is the row vector formed from the wave functions $\varphi_i^0(x)$

$$\varphi^0 = (\varphi_1^0, \varphi_2^0, \ldots \varphi_g^0), \qquad (3')$$

E is a diagonal matrix

$$E = \begin{pmatrix} E_1 & & & & \\ & E_2 & & & \\ & & \cdot & & \\ & & & \cdot & \\ & & & & \cdot \\ & & & & & E_g \end{pmatrix} . \qquad (3'')$$

The spin variable has been denoted by σ and the spin functions corresponding to the two possible spin states by χ_+ and χ_- respectively. f and g are defined in the following manner

$$f = \frac{n - q}{2}, \qquad g = \frac{n + q}{2},$$

where $q = 0$ if n is even and $q = 1$ if n is odd. If n is even $f = g$ and the term with index g in wave function (2) should of course be omitted. The spin function of the g-th state may be either χ_+ or χ_-, this being indicated by the index $\pm$ of the spin function.

Substituting the wave function Φ in (2) into equation (1) the energy eigenvalue of the system is

$$\mathscr{E} = 2 \sum_{i=1}^{g} E_i - q E_g . \qquad (4)$$

The wave functions φ_i^0 are orthogonal as they are the eigenfunctions belonging to various eigenvalues of the same operator. This is indicated by the index 0.

By direct substitution we find that equation (1) can also be satisfied by such a wave function

$$\Phi = \begin{vmatrix} \varphi_1 (x_1) \chi_+ (\sigma_1) \ldots \varphi_1 (x_n) \chi_+ (\sigma_n) \\ \varphi_1 (x_1) \chi_- (\sigma_1) \ldots \varphi_1 (x_n) \chi_- (\sigma_n) \\ \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \\ \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \\ \varphi_f (x_1) \chi_+ (\sigma_1) \ldots \varphi_f (x_n) \chi_+ (\sigma_n) \\ \varphi_f (x_1) \chi_- (\sigma_1) \ldots \varphi_f (x_n) \chi_- (\sigma_n) \\ \varphi_g (x_1) \chi_\pm (\sigma_1) \ldots \varphi_g (x_n) \chi_\pm (\sigma_n) \end{vmatrix}, \qquad (5)$$

the elements of which statisfy the equation

$$H \varphi (x) = \varphi (x) \in ,$$ (6)

where

$$\varphi = (\varphi_1, \varphi_2 \ldots, \varphi_g)$$ (6')

and

$$\in = \begin{pmatrix} \in_{11} \ldots, \in_{1g} \\ \ldots \ldots \ldots \\ \in_{g1} \ldots, \in_{gg} \end{pmatrix} .$$ (6")

Equations (3), (3'), (3'') correspond to the special case of equations (6), (6'), (6'') where the matrix $\in$ is diagonal, i. e. the one-particle wave functions are orthogonal to one another.

The eigenvalue now is

$$\mathscr{E} = 2 \sum_{i=1}^{g} \in_{ii} - q \in_{gg}.$$ (4')

At the same time it is obvious that the wave functions (2) and (5) can differ but by a proportionality factor. From this follows that between the one-particle wave function systems φ^0 and φ the following linear relation must exist

$$\varphi^0 = \varphi C ,$$

$$\varphi_i^0 = \sum_{k=1}^{g} \varphi_k C_{ki} .$$

As the components of both the vectors φ^0 and φ are linearly independent, C cannot be singular, i. e. there also exists the inverse transformation

$$\varphi = \varphi^0 C^0,$$

$$\varphi_i = \sum_{k=1}^{g} \varphi_k^0 C_{ki}^0.$$ (7)

C^0 denotes the reciprocal of the matrix C.

It is suitable to take the wave functions φ_i^0 and φ_i as normalized to 1. Further, as is known, in the case of a bound state the wave functions φ_i^0 and φ_i can be regarded as real without restricting the generality. Thus

$$\int \varphi_i^0 \varphi_k^0 \, dx = \delta_{ik}$$

and

$$\int \varphi_i^2 \, dx = 1 .$$

Now equation (7) immediately gives

$$\sum_{k=1}^{g} C_{ki}^{02} = 1$$

and

$$C_{ki}^{0} = \int \varphi_k^0(x') \, \varphi_i(x') \, dx'.$$

Apply transformation (7) to equation (3):

$$H \varphi(x) = \varphi(x) \, C \, E \, C^0.$$

Comparing this equation with equation (6) we obtain:

$$\epsilon = C \, E \, C^0.$$

Using this transformation equation (6) takes the following form

$$(H + O_i) \, \varphi_i(x) = E_i \, \varphi_i(x). \tag{8}$$

O_i may appear in the concrete form of e. g. an integral operator

$$O_i \varphi_i(x) = \int \sum_{k=1}^{g} (E_i - E_k) \, \varphi_k^0(x') \, \varphi_k^0(x) \, \varphi_i(x') \, dx',$$

or, what is essential for our considerations below, it can also be written in the form

$$O_i = \frac{1}{2\,m} (p_i^2 - \pi_i^2), \tag{9}$$

where p_i^2 and π_i^2 are the quantities defined by equations

$$- \hbar^2 \frac{d^2 \varphi_i^0(x)}{dx^2} = p_i^2(x) \, \varphi_i^0(x) \tag{9'}$$

and

$$- \hbar^2 \frac{d^2 \varphi_i(x)}{dx^2} = \pi_i^2(x) \, \varphi_i(x) \tag{9''}$$

respectively.

Substituting the form (9) of O_i into equation (8) after rearrengement we may cancel by $\varphi_i(x)$ and obtain for wave functions $\varphi_i^0(x)$ the equation (3). Thus if O_i is expressed in the form (9) equation (8) is a trivial transformation of (3). However, as we shall see later, with some further conditions on the wave functions φ_k $\quad (p_i^2 - \pi_i^2)/2m$ can be expressed in a semi-classical approximation by the wave functions φ_k, i. e. in such an approximation equations (8) and (9) can still be used for the determination of a non-orthogonal one-particle wave function system φ.

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For the following we shall need the expression of the density. The density of the i-th particle is by definition

$$\nu(x) = \frac{\int |\Phi(x_1, \ldots, x_{i-1}, x, x_{i+1}, \ldots, x_n)|^2 \, dx_1 \ldots dx_{i-1} \, dx_{i+1} \ldots dx_n}{\int |\Phi|^2 \, dx_1 \ldots dx_n}$$

and, as Φ is antisymmetrical, $\nu(x)$ is the same for any particle, the total density thus being

$$\varrho(x) = n\,\nu(x). \tag{10}$$

In the case of orthogonal one-particle wave functions the integration can readily be carried out and the following result is obtained

$$\varrho(x) = 2\sum_{i=1}^{g}{}' \varphi_i^{0\,2}(x) - q\,\varphi_g^{0\,2}(x). \tag{10'}$$

To the energy expression (4) and the density expressions (10') the following meaning can be attributed. We may imagine the particles of the system to fill the one-particle states characterized by the wave functions φ_i^0 and the energy eigenvalues E_i and the respective sums of the densities and energies of the particles thus distributed give the density and energy of the system. It must be emphasized that this is only to illustrate the situation as in reality the densities of the individual particles are identical and according to (10) they are equal to the n-th part of the total density.

Let us investigate the situation from this standpoint, in the case of non-orthogonal one-particle wave functions. The expression (10') of the density remains unchanged if

$$2\sum_{i=1}^{g}{}' \varphi_i^{0\,2}(x) - q\,\varphi_g^{0\,2}(x) = 2\sum_{i=1}^{g}{}' \varphi_i^2(x) - q\,\varphi_g^2(x).$$

Then, provided that n is even, the transformation the matrix of which is C or C^0 is orthogonal. This means, however, that wave functions φ_i also form an orthonormalized system of functions which contradicts our assumption. If n is odd, but sufficiently large, the wave-functions φ_i become quasi-orthogonal, which is also incompatible with the following.

This problem can be solved if the wave functions satisfy the following conditions

a) the wave functions φ_i should be everywhere positiv nodeless wave-functions.

b) the densities $\nu_i = \varphi_i^2$ should average the densities $\nu_i^0 = \varphi_i^{0\,2}$ as well as possible. (Thus e. g. $\nu_1 = \nu_1^0$) Between the wave functions φ_i and φ_i^0 the linear transformation (7) must exist. The matrix components of C^0 should be chosen so that, in addition to satisfying condition *a)*, the values of the

integrals of v_i and v_i^0 agree for the subsequent intervals. (These intervals are first of all determined by the nodes of wave-function φ_i^0. If $i < g$ limits for these intervals can also be designated between these nodes which are suitable to assume where the two neighbouring nodes are far from each other.)

Thus the function

$$N(x) = 2 \sum_{i=1}^{g} v_i - q\, v_g \tag{10''}$$

averages the density ϱ well and in the following can also be regarded as a density. Thus, with regard to equation (8) the visualizing idea that the energy and the density of one-particle states can be regarded as the energy and density, respectively of the individual particles can be maintained in the case of the non-orthogonal one-particle wave function system φ.

The necessity of condition $a)$ will be shown below.

3. Semiclassical approximation

Consider what the semi-classical analogue of the expression (9) of O_i is. Applying the first approximation of the WKB method $p_i^2/2m$ is the kinetic energy of the particle in the i-th state thus

$$2 \int_{x_1(E_i)}^{x_2(E_i)} p_i\, dx = (i - 1/2)\, h\,, \tag{11}$$

where

$$p_i = \left[2\, m\, (E_i - V(x)) \right]^{1/2} \tag{11'}$$

and $x_1(E_i)$ and $x_2(E_i)$ are the classical turning points.[1]

Introduce the notation

$$P_i = (p_i + p_{i+1})/2\,. \tag{12}$$

P_i can be regarded as the maximum momentum of the particles occupying the quantum states of energy lower than that of the $(i + 1)$-th quantum state. The density of these particles be denoted by

$$N_i = 2 \sum_{k=1}^{i} v_k. \tag{12'}$$

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[1] Here E_i means the eigenvalue obtained in the WKB approximation, whereas in the preceding chapter E_i detoned the exact eigenvalue. In the following the exact eigenvalue as well as the eigenvalues obtained in the various approximations will be detoned by E_i. In the case where this might lead misunderstanding special reference will be made.

As a first approximation of the WKB method the well-known statistical relation can be derived:

$$P_i = \frac{h}{4} N_i \,. \tag{13}$$

We note that in a former paper [9] this relation was improved to distinguish between systems consisting of an even or odd number of particles. Thus for the g-th state:

$$P = \frac{h}{2} \frac{}{n} N \,. \tag{13'}$$

Here the notation $Pg = P$ has been introduced. If n is even (13') goes over into (13). (Then $N = Ng$.)

ν_i can be written in the form

$$\nu_i = \frac{1}{2} (N_i - N_{i-1}) = \frac{2}{h} (P_i - P_{i-1}) \tag{14}$$

By relation (11')

$$p_{i+1}^2 - p_{i-1}^2 = 2\,m\,(E_{i+1} - E_{i-1}),$$
$$(i \geq 2)$$

based on which and using (12), (13) and (14) we obtain

$$\nu_i = \frac{m\,(E_{i+1} - E_{i-1})}{h} \frac{1}{p_i'} \,,$$
$$(i \geq 2) \tag{14'}$$

where

$$p_i' = (p_{i+1} + p_{i-1})/2 \,.$$

With this, according to equation (9'') taking the condition a) at the end of the previous chapter into account

$$\frac{1}{2\,m} \pi_i^2 = -\frac{\hbar^2}{2\,m} p_i'^{1/2} \frac{d^2\,p_i'^{1/2}}{dx^2} \,,$$
$$(i \geq 2)$$

which in the region $V < E_i$

$$O_i = \frac{1}{2\,m} p_i^2 + \frac{\hbar^2}{2\,m} p_i'^{1/2} \frac{d^2\,p_i'^{-1/2}}{dx^2} \,,$$
$$(i \geq 2) \tag{15}$$
$$O_1 \equiv 0, \text{ as } p_1^2 \equiv \pi_1^2 \,.$$

To evaluate this let us consider the following.

MILNE [10] suggests the following way to determine the eigenvalues

$$2 \int_{-\infty}^{\infty} P' \, dx = i \, h, \tag{16}$$

where P_i' satisfies the following second order differential equation

$$\frac{1}{2 \, m} P_i'^2 - \frac{\hbar^2}{2 \, m} P_i'^{1/2} \frac{d^2 \, P_i'^{-1/2}}{dx^2} + V(x) = E_i. \tag{16'}$$

The similarity between the equations of Milne's method and those of the WKB method is striking, an essential difference, however, is that MILNE's method is exact (E_i is the exact eigenvalue). Comparing equation (16') with (11') we see that in the WKB approximation, in which case the eigenvalues E_i in the equations (16') and (11') agree, p_i and P_i' must be related in the redion $V < E_i$ in the following manner

$$\frac{1}{2 \, m} p_i^2 = \frac{1}{2 \, m} P_i'^2 - \frac{\hbar^2}{2 \, m} P_i'^{1/2} \frac{d^2 \, P_i'^{-1,2}}{dx^2} \, . \tag{17}$$

Assumption (16) makes very plausible that the function P_i' and the momentum P_i in (13) may be taken as approximately equal. This relation has been shown by Plaskett [7].

Assuming further that

$$P_i^{1/2} \frac{d^2 P_i^{-1/2}}{dx^2} = p_i^{1/2} \frac{d^2 p_i^{-1/2}}{dx^2} = p_i'^{1/2} \frac{d^2 p_i'^{-1/2}}{dx^2}, \tag{17'}$$

we obtain from (17) and (15) that in the region $V < E_i$

$$O_i = \frac{1}{2 \, m} P_i^2 = \frac{h^2}{32 \, m} N_i^2,$$

$$(i \geq 2) \tag{15'}$$

$$O_1 \equiv 0$$

In the region $V > E_i$ $O_i = 0$ as here the wave functions φ_i^0 and φ_i can be taken as approximately equal by conditions $b)$ of the previous chapter, since in this region the function φ_i^0 has no node.

By substituting this form of O_i into equation (8) we obtain a system of equations from which the wave-functions φ_i and the eigenvalues E_i can actually be determined :

$$-\frac{\hbar^2}{2\,m}\frac{1}{\nu_i^{1/2}}\frac{d^2\,\nu_i^{1/2}}{dx^2} + \frac{1}{2\,m}P_i^2 + V = E_i\,,(V < E_i),\qquad(8')$$

$$-\frac{\hbar^2}{2\,m}\frac{1}{\nu_i^{1/2}}\frac{d^2\,\nu_i^{1/2}}{dx^2} + V = E_i\,,\;(V > E_i)\,,\qquad(8'')$$

$$(i \gtrless 2)$$

$$-\frac{\hbar^2}{2\,m}\frac{1}{\nu_1^{1/2}}\frac{d^2\,\nu_1^{1/2}}{dx^2} + V = E_1\,.$$

For the following the relation of equation (8′) to PLASKETT's equation is essential. Substituting in equation (8′) the approximation (14′) of ν_i valid for the region $V < E_i$ and using (17′)

$$-\frac{\hbar^2}{2\,m}N_i^{1/2}\frac{d^2\,N_i^{-1/2}}{dx^2} + \frac{1}{2\,m}P_i^2 + V = E_i,\;(V < E_i).\qquad(16'')$$

$$(i \gtrless 2)$$

However, in the region $V > E_i$ the assumption can be allowed that ν_i is proportional to N_i as, if $V \gg E_i$ ν_i is practically identical with N_i. Thus according to equation (8″),

$$-\frac{\hbar^2}{2\,m}N_i^{-1/2}\frac{d^2\,N_i^{1/2}}{dx^2} + V = E_i,\;(V > E_i).\qquad(16''')$$

Plaskett's equation is obtained by replacing P'_i in equation (16′) by P_i in (13). The equation thus obtained agrees with (16″) it does not, however, involve the restriction that the equation is valid only for the region $V < E_i$. In deriving form (15′) of O_i Plaskett's equation has been used and the first approximation of the WKB method has been applied. Thus one term of equation (8′) also contains these approximations. Equation (8″) is free of them as it can be regarded as the direct consequence of the fact that in the region $V > E_i$ the wave functions φ_i^0 and φ_i are approximately equal. Equation (16″), which is the approximation of equation (8′) is identical with Plaskett's while equation (16‴) is, according to above, certainly more accurate in the region $V > E_i$ than Plaskett's equation. We may thus conclude that equations (16″) and (16‴) are the improved versions of Plaskett's equation.

BALLINGER and MARCH [11] investigated the solution of Plaskett's equation in the case of an oscillator potential and found that the solution is not unique. According to the above, however, we must proceed in such a manner that the solution of equation (16″) obtained in the region $V < E_i$ must be fitted to the solution of equation (16‴) obtained in the region $V > E_i$. The fitting is a new condition for the solution of equation (16″) whereby the solution is likely to become unique.

The question arises whether an equation could be found from which the density could be determined for the whole space. Assume that in the region $V < E_i$ the densitiy is large as compared to the variation of the density. Then we have

$$N_i^{-1/2} \frac{d^2 N_i^{1/2}}{dx^2} = - N_i^{1/2} \frac{d^2 N_i^{-1/2}}{dx^2}$$

ni equation (16") can be written in the form

$$- \frac{\hbar^2}{2\,m} N_i^{-1/2} \frac{d^2 N_i^{1/2}}{dx^2} + \frac{1}{2\,m} P_i^2 - \frac{\hbar^2}{m} P_i^{1/2} \frac{d^2 P_i^{-1/2}}{dx^2} + V = E_i.$$

Applying (17) and (17')

$$\frac{1}{2\,m} P_i^2 - \frac{\hbar^2}{m} P_i^{1/2} \frac{d^2 P_i^{-1/2}}{dx^2} = \frac{1}{2\,m} p_i^2 - \frac{\hbar^2}{2\,m} p_i^{1/2} \frac{d^2 p_i^{-1/2}}{dx^2},$$

further, by generalizing relation (17) to some extent

$$\frac{1}{2\,m} p_i^2 - \frac{\hbar^2}{2\,m} p_i^{1/2} \frac{d^2 p_i^{-1/2}}{dx^2} = \frac{1}{2\,m} P_{i-1}^2.$$

Thus

$$- \frac{\hbar^2}{2\,m} N_i^{-1/2} \frac{d^2 N_i^{1/2}}{dx^2} + \frac{1}{2\,m} P_{i-1}^2 + V = E_i. \tag{18}$$

If $i = 1$ this equation goes over into the exact wave mechanical equation, further, if $V > E_i$ into equation (16 "), since, in this case, $P_{i-1}^2/2\mathrm{m}$ can be neglected. Thus equation (18) can be regarded as valid for all states and the whole space.

4. The statistical energy expression

Starting from equation (18) a further approximation makes it possible to express the energy of the system with the aid of the particle density of the system. The energy value E_i is obtained by multiplying equations (18) by $N_i/2i$ and by integrating over the whole space. The total energy is obtained by summation according to (4)

$$\mathscr{E} = \sum_{i=1}^{g} \frac{1}{i} \left\{ - \frac{\hbar^2}{2\,m} \int N_i^{1/2} \frac{d^2 N_i^{1/2}}{dx^2}\, dx + \frac{h^2}{32\,m} \int N_{i-1}^2 N_i\, dx + \int N_i\, V\, dx \right\} -$$

$$- \frac{q}{2\,g} \left\{ - \frac{\hbar^2}{2\,m} \int N_g^{1/2} \frac{d^2 N_g^{1/2}}{dx^2}\, dx + \frac{h^2}{32\,m} \int N_{g-1}^2 N_g\, dx + \int N_g\, V\, dx \right\}.$$

Introduce the approximation that $N_i = \dfrac{2\,i}{n}\,N$. Then the energy expression is

$$\mathscr{E} = \mathscr{E}_W + \mathscr{E}_K + \mathscr{E}_P \qquad (19)$$

where

$$\mathscr{E}_W = -\frac{h^2}{2\,m}\int N^{1/2}\frac{d^2\,N^{1/2}}{dx^2}\,dx = \frac{h^2}{8\,m}\int\frac{1}{N}\left|\frac{d\,N}{dx}\right|^2 dx\,,$$

$$\mathscr{E}_K = \frac{h^2}{8\,m\,n^3}\left[\frac{(g-1)\,g\,(2g-1)}{3} - q\,(g-1)^2\right]\int N^3\,dx\,,$$

$$\mathscr{E}_p = \int V\,N\,dx.$$

Obviously $\mathscr{E}_W$ is just the energy which is generally called the Weizsäcker inhomogeneity correction. It is suitable to compare the kinetic energy $\mathscr{E}_K$ with the Fermi zero point kinetic energy. The expression for the zero point kinetic energy has been improved upon in a previous paper [9] in such a manner that — under condition similar to those of the present paper — instead of integrating over the momentum space we summed over the states exactly

$$\mathscr{E}_0 = \frac{h^2}{8\,m\,n^3}\left[\frac{g\,(4\,g^2-1)}{6} - q\,(g-1/2)^2\right]\int N^3 dx.$$

Comparing the expressions of $\mathscr{E}_K$ and $\mathscr{E}_0$ we have

$$E_K = t\,\mathscr{E}_0$$

where

$$t = \frac{2\,(g-1)\,g\,(2\,g-1) - 6\,q\,(g-1)^2}{g\,(4\,g^2-1) - 6\,q\,(g-1/2)^2}$$

or in a different manner

$$t = \frac{n-2}{n+1}\ \ \text{if } n \text{ is even,}$$

$$t = \frac{(n-1)\,\left[(n-1)^2+2\right]}{n\,\left[n^2+2\right]}\ \ \text{if } n \text{ is odd.}$$

If the number of particles is 1 or 2, $\mathscr{E}_K = 0$ thus here the total kinetic energy is represented by the Weizsäcker correction only and the relations go over into the exact wave mechanical expressions.

The fact that in the satistical theory the zero point kinetic energy should be decreased when the Weizsäcker correction is incorporated in the theory was first pointed out by GOMBÁS [6]. His method was confirmed by his calculations for atoms.

5. Determination of the density

The statistical equation determining the density can be obtained by searching for the density for which $\mathscr{E}$ is a minimum. Elementary calculation yields

$$-\frac{\hbar^2}{2m}\frac{1}{N^{1/2}}\frac{d^2 N^{1/2}}{dx^2} + \frac{1}{2mn}\frac{1}{g^2}[(g-1)g(2g-1) - 3q(g-1)^2]P^2 + V = V_0,$$
(19')

where V_0 is the Lagrange multiplicator.

The determination of the density is more accurate if the following procedure is applied. Let us write equations (16'') and (16''') for the g-th state. Take into account that $P_g = P$ and if n is even $N_g = N$ and if n is odd, we may use the approximation $N_g = \dfrac{2g}{n}N$,

$$-\frac{\hbar^2}{2m}N^{1/2}\frac{d^2 N^{-1/2}}{dx^2} + \frac{1}{2m}P^2 + V = E_g, \quad (V < E_g),$$
(20)

$$-\frac{\hbar^2}{2m}N^{-1/2}\frac{d^2 N^{1/2}}{dx^2} + V = E_g, \quad (V > E_g).$$
(20')

Instead of using equation (20) of Plaskett we may also proceed in the following manner. Equation (8') for the g-th state is

$$-\frac{\hbar^2}{2m}\frac{1}{\nu_g^{1/2}}\frac{d^2 \nu_g^{1/2}}{dx^2} + \frac{1}{2m}P^2 + V = E_g, \quad (V < E_g).$$
(21)

Calculate the density from equation (19') for the case when the number of particles of the system is n and $n-1$ resp. The difference between these two will yield approximately ν_g. Knowing ν_g and using (13') from equation (21) we may express N

$$N = \frac{2}{h}\frac{n}{g}\left\{2m\left|E_g - V + \frac{\hbar^2}{2m}\frac{1}{\nu_g^{1/2}}\frac{d^2 \nu_g^{1/2}}{dx^2}\right|\right\}^{1/2}, \quad (V < E_g).$$
(21')

Equation (20) and (21') are both approximations of equation (21).

In conclusion it should be mentioned that for a large number of particles we may obtain from (21) a partial differential equation for N as the continuous function of the number of particles. Regarding N as the derivable function of the number of particles, then $\nu_g = \displaystyle\int_{n-1}^{n}\frac{\partial N}{\partial k}\,dk$ and if n is large $\nu_g = \dfrac{\partial N}{\partial n}$ which

substituted into equation (21) yields that

$$-\frac{\hbar^2}{4\,m}\frac{\partial N}{\partial n}\frac{\partial^3 N}{\partial x^2 \partial n}+\frac{\hbar^2}{8\,m}\left(\frac{\partial^2 N}{\partial x\,\partial n}\right)^2+\frac{\hbar^2}{8\,m}\frac{g^2}{n^2}N^2\left(\frac{\partial N}{\partial n}\right)^2+$$

$$+V\left(\frac{\partial N}{\partial n}\right)^2=E_g\left(\frac{\partial N}{\partial n}\right)^2,\ (V<E_g).$$

Similarly, starting form equation (8″) assumed for the g-th state

$$-\frac{\hbar^2}{4\,m}\frac{\partial N}{\partial n}\frac{\partial^3 N}{\partial x^2 \partial n}+\frac{\hbar^2}{8\,m}\left(\frac{\partial^2 N}{\partial x\,\partial n}\right)^2+V\left(\frac{\partial N}{\partial n}\right)^2=E_g\left(\frac{\partial N}{\partial n}\right)^2,$$

$$(V>E_g).$$

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О СТАТИСТИЧЕСКОЙ ТРАКТОВКЕ ФЕРМИОН-ГАЗА

П. СЕПФАЛУШИ

Резюме

Выводится новая статистическая модель, которая в большой мере подобна видоизмененной Гомбашем модели Вайцсеккера, дополненной поправкой на неоднородность. При введенных приближениях суммирование по квантовым состояниям не надо аппроксимировать интегрированием, а можно произвести точно. Кроме определения плотности из вариационного принципа, показаны и более точные методы расчета. Доказывается, что плотность из уравнений Пласкета можно определить только в рамках «классически допустимой области» и выводится соответствующие уравнение на «запрещенную область».