CONDITIONS FOR THE APPLICABILITY OF STATISTICAL FORMULAS TO A DEGENERATE FERMI GAS

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A degenerate ideal Fermi gas in an arbitrary potential field is considered. It is shown that a sufficient condition for the applicability of statistical formulas to the problem of the change of the density under the action of the potential $V(\mathbf{r})$ is that the motion of the particles with the maximum (Fermi limit) energy be a quasiclassical motion. This result is not invalidated by nonapplicability of the quasiclassical approximation to the motion of particles with smaller energies, and in particular, for $V < 0$, to that of bound particles. The corrections to the statistical formulas in the one-dimensional and three-dimensional problems have opposite signs.

1. INTRODUCTION

WE shall examine the limits of applicability of the well known expressions for the density of a degenerate Fermi gas with boundary energy $\mathscr{E}$, in a potential field $V(\mathbf{r})$, for particles of spin $\frac{1}{2}$:

$$\rho_1 = 2K_m/\pi, \quad \Delta\rho_1 = \rho_1 - \rho_{10} = (2\sqrt{2}/\pi)\,[(\mathscr{E}-V)^{1/2} - \mathscr{E}^{1/2}] \tag{1.1}$$

in the one-dimensional case and

$$\rho_3 = \frac{8\pi}{3}\left(\frac{K_m}{2\pi}\right)^3, \quad \Delta\rho_3 = \frac{2\sqrt{2}}{3\pi^2}\,[(\mathscr{E}-V)^{3/2} - \mathscr{E}^{3/2}] \tag{1.2}$$

in the three-dimensional case, where K_m is the local boundary wave number (we take $\hbar = m = 1$)

$$K_m(\mathrm{r}) = \sqrt{2(\mathscr{E} - V(\mathrm{r}))}. \tag{1.3}$$

The textbook derivation of these expressions involves counting up the numbers of states per unit volume in regions with given values of $V(\mathbf{r})$. Let us think of a case with $V(\mathbf{r})$ negative in a restricted region of space and zero everywhere outside this region (potential well). Then it would seem that for the applicability of the formulas it is necessary for a large number of particles to be bound in the well. The question presents itself particularly sharply in the one-dimensional case. For $V \ll \mathscr{E}$ we find

$$\Delta\rho_1 = -\sqrt{2}V/\pi\sqrt{\mathscr{E}}. \tag{1.4}$$

For definiteness let us consider a well, i.e., the case $V < 0$, $\Delta\rho_1 > 0$. With increase of $\mathscr{E}$ the total change of the density of the gas over the well decreases. The meaning of this result is clear: in the one-dimensional case the well always has at least one bound level with $E < 0$, which makes a positive contribution to $\Delta\rho_1$. The free particles with $E > 0$ travel more rapidly when over the well than elsewhere, and consequently their density over the well is smaller. Therefore the quantity $\Delta\rho_1$ is the difference of the positive contribution of the bound particles (independent of $\mathscr{E}$) and the negative contribution of the free particles with $0 < E < \mathscr{E}$.

Can the formula be applied when there is a single bound state? For small $|V|$ the bound particle is localized in a region much larger than the well itself. What is the localization of $\Delta\rho_1$ in this case?

As will be shown below (Sec. 2), in the one-dimensional case the tendency of $\Delta\rho_1$ to zero as $\mathscr{E} \to \infty$ is an exact quantum-mechanical theorem, i.e., it is valid independently of the applicability of the statistical formula (1.4). This theorem is connected with the completeness of the system of eigenfunctions, both that in the unperturbed case ($V = 0$; ψ_0), and also the system of eigenfunctions in the field $[V(x); \psi_n]$; from this property we have

$$\int_{-\infty}^{+\infty} |\psi_0(x, E)|^2\,dE = \int_{-\infty}^{+\infty} |\psi_n(x, E)|^2\,dE$$

(the integral is taken in the Stieltjes sense, including the discrete levels).

As a result of this theorem, the change of the density that comes from the inclusion of the particles with energies smaller than $\mathscr{E}$ is equal in magnitude and opposite in sign to the change of the density of all the particles with energies larger than $\mathscr{E}$.

If the quasiclassical approximation is valid for

the particles with energies equal to and greater than E in the field V(x), then from this it is easy to get the expression (1.4). Thus the expressions (1.1) and (1.4) can be obtained independently of the number of bound levels and of the character of the motion of the particles with energies less than $\mathcal{E}$. This argument also provides an approach (Sec. 3) to an estimate of the accuracy of Eqs. (1.1) and (1.4). In fact, considering the particles with energies larger than $\mathcal{E}$, we convince ourselves that for small V

$$\Delta\rho_1(x) = \int L(|x-y|)\,V(y)\,dy; \qquad (1.5)$$

the function $L(|x-y|)$ is different from zero in an interval of the order of $1/K_m$, where K_m is the wave number corresponding to the boundary energy $\mathcal{E}$.

The smearing out described by the function $L(|x-y|)$ does not change the total increase of the number of particles in the neighborhood of the region of action of the potential, and from Eq. (5) one gets

$$\int \Delta\rho_1(x)\,dx = -\frac{\sqrt{2}}{\pi\sqrt{\mathcal{E}}}\int V(x)\,dx \qquad (1.6)$$

in exact agreement with Eq. (1.4).

The deviation from the formula (1.6) is of higher order in V(x), whereas the deviations from the local formula (1.4) are of first order in V(x) and are due to the spatial distribution of V(x). Together with the leading correction term the expression (1.6) has the form [cf. Eq. (1.1)]

$$\int \Delta\rho_1(x)\,dx = 2\sqrt{2}\pi^{-1}\int[(\mathcal{E}-V)^{1/2} - \mathcal{E}^{1/2}]\,dx + b\mathcal{E}^{-1/2}\int (dV/dx)^2\,dx.$$

Let us turn to the three-dimensional case (Sec. 4). From Eqs. (2) and (3) we get for small V

$$\Delta\rho_3 = -\sqrt{2}\pi^{-2}V(\mathbf{r})\,\mathcal{E}^{1/2}.$$

This expression increases without bound with increasing $\mathcal{E}$; from this it follows that for large $\mathcal{E}$ the main contribution comes from the change of the density of the free particles.

In the limit of small V the quantum-mechanical problem of the perturbation of the density of a plane wave is easy to solve in the Born approximation. Summing the contributions of all plane waves with energies smaller than E, we get the answer in the form

$$\Delta\rho_3(\mathbf{r}) = \int M(|\mathbf{r}-\mathbf{r}'|)\,V(\mathbf{r}')\,d\mathbf{r}'.$$

The function M found in this way also falls off at a distance of the order of $1/K_m$.

As is well known, in the three-dimensional case a sufficiently small well does not have any bound state at all. The application of the general arguments associated with the completeness of the system of eigenfunctions to the three-dimensional case requires an extremely careful definition of the procedure of passage to the infinite limit; thus this method is not an effective one. If, however, we have three-dimensional motion with a potential that allows separation of variables, for example a V(r) independent of θ and φ, or a V(x) independent of y and z, the completeness theorem can be unconditionally applied to each group of particles with fixed values of the conserved quantities — the angular momenta in the case of V(r), or k_y, k_z in the case of V(x). The completeness theorem then enables us to carry out the most difficult part of the calculation — the summation over k_r or k_x — by going over to the range of energies above the boundary energy and using the quasiclassical approximation. All told, by using different methods in the one-dimensional and three-dimensional problems, we are able in both cases to get an idea of the degree of accuracy of the statistical formulas and of the difference between the statistical expressions and the exact quantum-mechanical solutions.

The main result is that everything depends on the quasiclassical character of the motion of the particles with the boundary energy $\mathcal{E}$. For small V this result is a natural one, if we deal directly with the many-particle problem in the Fock representation in which the unperturbed eigenfunctions are antisymmetrized products, that is, Slater determinants, of plane waves. In such a treatment any perturbation V (including in particular a potential that has bound states) only causes transitions of the particles from the region $E < \mathcal{E}$ into the region $E > \mathcal{E}$. It seems to us, however, that only the examination we have made of the change of the one-particle states gives a completely intuitive picture of the realization of the statistical laws, and in particular gives a possibility of passing on easily to the case of a V that is comparable with the boundary energy $\mathcal{E}$, for which one cannot use just first-order perturbation theory.

2. THE COMPLETENESS THEOREM IN THE ONE-DIMENSIONAL PROBLEM

Let us consider the motion of particles in a field V(x) that has the eigenfunctions $\psi_n(x)$,

including both a discrete and a continuous spectrum.

Let us add to the potential a small perturbation δV (with arbitrary dependence on x) and find the changes of $\psi_n(x)$ and $\rho_n(x) = |\psi_n(x)|^2$ by first-order perturbation theory. To abbreviate the writing let us consider real nondegenerate functions; it is easy to verify that the results do not depend on this.

$$\delta\psi_n = \sum_m{}' \frac{\psi_m}{E_n - E_m} V_{mn}, \qquad \delta\rho_n(x) = \sum_m{}' A_{nm}(x), \quad (2.1)$$

$$V_{mn} = \int \psi_m(x)\,\delta V(x)\,\psi_n(x)\,dx, \qquad A_{nm} = \frac{2\psi_n\psi_m V_{mn}}{E_n - E_m}. \quad (2.2)$$

Let the index n be monotonically related to the energy. We consider the total change of the density of all the particles with $n < \nu$,

$$\delta\rho(n<\nu) = \sum_n^{\nu}\delta\rho_n = \sum_n^{\nu}\sum_m{}' A_{nm}. \quad (2.3)$$

We now make use of the fact that A_{nm} is antisymmetric, $A_{nm} = -A_{mn}$. Because of this the sum over all n from 0 to ∞ is identically zero. This means that

$$\delta\rho(n<\nu) + \delta\rho(n>\nu) = 0,$$
$$\delta\rho(n<\nu) = -\delta\rho(n>\nu) = -\sum_{n=\nu}^{\infty}\delta\rho_n. \quad (2.4)$$

Since Eq. (2.4) holds for an arbitrary small variation $\delta V(x)$, with an arbitrary and not small $V(x)$, the same relation also holds for an arbitrary change of $V(x)$, in particular for the change of $V(x)$ from 0 to a given final $V(x)$.

For $V = 0$, $\rho(x) = \text{const} = \rho_0$, and consequently

$$\Delta\rho(n<\nu) = -\sum_{n=\nu}^{\infty}[\rho_n(x) - \rho_{0n}(x)]. \quad (2.5)$$

The meaning of this transformation is that the sum over $n < \nu$ gives the essential contribution of the discrete states, and also the contribution of states for which E is small and the wavelength is large; for each of these states individually a potential $V(x)$ that is different from zero in a small region of space causes changes of $\psi_n(x)$ and $\rho_n(x)$ at large distances, of the order of a wavelength.

By using Eq. (2.5) we go on to the examination of particles with energies larger than the boundary energy $\mathscr{E} \equiv E_\nu$. For particles with $E > \mathscr{E}$ the condition for the quasiclassical nature of the motion in the field $V(x)$ is much less restrictive. If it is satisfied, then for wave functions normalized in unit volume we have

$$\psi(x) = \sqrt{k_0/k}\exp\left\{i\int k\,dx\right\}, \qquad k(x) = \sqrt{k_0^2 - 2V(x)}, \quad (2.6)$$
$$\rho(x) - \rho_0 = -(k - k_0)/k_0, \quad (2.7)$$
$$\Delta\rho(k<k_m) = \frac{2}{\pi}\int_{k_m}^{\infty}\frac{k-k_0}{k_0}\,dk_0. \quad (2.8)$$

From this we find

$$\Delta\rho(k<k_m) = 2(k_m - k_{m0})/\pi. \quad (2.9)$$

The unperturbed density is $\rho_0 = 2k_{0m}/\pi$, so that

$$\rho(k<k_m) = (2/\pi)\sqrt{k_0^2 - 2V} = 2k_m/\pi.$$

Thus the first point of the program stated in the introduction has been accomplished: an expression that agrees with the elementary formula (1.1) has been derived on the single assumption that the motion of particles whose energy exceeds the boundary energy is quasiclassical, although in reality we have to do with an assembly of particles whose energies are less than the boundary value, and whose motions may not be quasiclassical.

3. THE CORRECTIONS TO THE STATISTICAL FORMULA

To find the deviations from the elementary formulas (1.1) and (2.9) we can use two methods, in each of which we use the completeness theorem and make the calculations with wave functions for energies larger than the boundary energy.*

The first method is the use of the quasiclassical approximation

$$\psi_{k_0} = \sqrt{k_0/k}\exp\left\{-\sigma_3 + i\left[\int k\,dx - \sigma_2\right]\right\};$$
$$\sigma_2 = \frac{k'}{4k^2} + \frac{1}{8}\int\frac{k'^2}{k^3}\,dx, \qquad \sigma_3 = \frac{3}{16}\left(\frac{k'}{k^2}\right)^2 - \frac{k''}{8k^3}. \quad (3.1)$$

From this it follows that

$$\Delta\rho(k_0) = -\frac{2}{\pi}\int k_0\,dk_0\left[\frac{1}{k} - \frac{1}{k_0} - \frac{V''}{4k^5} - \frac{5V'^2}{8k^7}\right]. \quad (3.2)$$

Substituting in Eq. (2.5) and carrying out the integration, we get the answer in the form

$$\Delta\rho = \frac{2}{\pi}\left[\left(\sqrt{2(\mathscr{E}-V)} - \sqrt{2\mathscr{E}}\right) + \frac{V''}{12k_m^3} + \frac{V'^2}{8k_m^5}\right], \quad (3.3)$$

where the term in parentheses is the statistical formula, and the further terms give corrections to it. The problem of the quantum corrections to the statistical formulas has also been treated earlier by several writers.[1-3] We note that in the one-dimensional case the sign of the correction to the statistical formulas is opposite to that in the three-dimensional case (see Sec. 4 and references 1 — 3).

*For simplicity we confine ourselves to the case $V < \mathscr{E}$.

In the derivation of Eqs. (3.1) and (3.2) we neglect the amplitude of the reflected wave and consider only the deformation of the transmitted wave. As is well known, the amplitude of the reflected wave is proportional to the matrix element

$$\int V(x)\, e^{2ikx}\, dx. \tag{3.4}$$

For an analytic V(x) without singularities on the real axis this matrix element $\sim \exp\{-2k \operatorname{Im}(x_0)\}$, where $\operatorname{Im}(x_0)$ is the imaginary part of the coordinate x_0 of a pole of V(x). Such a term does not contribute to an expansion in powers of 1/k, and therefore the expansion (3.3) is only an asymptotic expansion.

The second method is the use of the Born approximation. For a V(x) that is of arbitrary form, but small, we find, again by using the completeness theorem,* that

$$\Delta\rho(k<k_m) = -\int_{k_m}^{\infty} dk \int_{-\infty}^{\infty} V(\xi)\, l(k, |x-\xi|)\, d\xi$$

$$= \int_{-\omega}^{+\infty} V(\xi)\, L(|x-\xi|)\, d\xi = \int_{k_m}^{\infty} j(x, k)\, dk,$$

$$L = \int l\, dk = -\frac{2}{\pi} \int_{2k_m |x-\xi|}^{\infty} \frac{\sin t}{t}\, dt,$$

$$j(x,k) = \frac{2}{\pi} \int_{-\infty}^{+\infty} V(x') \frac{\sin 2k\,|x-x'|}{|x-x'|}\, dx'. \tag{3.5}$$

We note that $l(y)$ and L(y) are even, but not analytic, functions; they have a singularity (discontinuity of all odd derivatives) at y = 0; therefore in the integral (3.5) the values of $V(\xi)$ at $x = \xi$ are singled out.

Equation (3.5) shows that $\Delta\rho$ is not zero outside the region of action of the potential, where V = 0. Then the integral

$$J = \int V(\xi)\, L(|x-\xi|)\, d\xi$$

comes entirely from the region where L has no singularities, and consequently according to the theory of the Fourier integral the value of J is determined by the singularities of V(x), the discontinuities of V(x) or of its derivatives and the poles of V(x) in the complex plane.

For example, if $V(x) = a\delta(x-x_0)$, then $\Delta\rho = aL(|x-x_0|)$, so that in the region where V = 0 and $\Delta\rho$ is zero by the statistical formula we actually have $|\Delta\rho| \sim 1/k_m x$; when there is a discontinuity of the derivative of V(x), $|\Delta\rho| \sim (k_m x)^2$, and so on.

The expression (3.5) brings out the fact that the scale of length in the solution is $\lambda_m = 1/k_m$, the wavelength of a particle moving with the boundary energy; on the other hand, the bound particles and low-energy particles, on which V(x) acts especially strongly, have $\lambda \gg \lambda_m$. Consequently, there is effective mutual compensation of their contributions.

We note in conclusion that the formulas become inapplicable when V(x) is small but has resonance properties, say $V \sim \sin k_m x$; as is well known, in this case the spectrum breaks up into zones; coincidence of a zone boundary with the boundary energy of the Fermi distribution decidedly changes the properties of the gas (in particular it turns a metal into a dielectric).

4. THREE-DIMENSIONAL MOTION

In the three-dimensional case a localized ($V(\mathbf{r}) = 0$ for $|\mathbf{r}| > R_0$) small potential V has no bound levels and the Born approximation applies for arbitrary energy, in particular for E < V, if $VR_0^2 \to 0$. For this reason we can do without the completeness theorem and integrate over the occupied states

$$\Delta\rho(\mathbf{r}) = \int L(k_m, R)\, V(\mathbf{r}')\, d\mathbf{r}',$$

$$L = \frac{\sin(2k_m R) - 2k_m R \cos(2k_m R)}{4R^4}. \tag{4.1}$$

Expanding $V(\mathbf{r})$ in a series in $\mathbf{r}-\mathbf{r}'$, we get the well known result

$$\Delta\rho = -\pi^{-2}\left(Vk_m + \frac{\nabla^2 V}{12k_m}\right). \tag{4.2}$$

The general character of the formulas (conservation of Δn, practical absence of effects at distances beyond $1/k_m$) does not differ from that of the corresponding formulas of the one-dimensional problem; the coefficient of V naturally correspond to the statistical formula. A nontrivial point, however, is the difference of the sign of the correction; in the one-dimensional case the coefficient of $\nabla^2 V$ was negative.

Let us now examine the special case of three-dimensional motion in a potential V = V(x). In this case k_y and k_z are integrals of the motion, and for fixed k_y and k_z, according to Eq. (3.3),

$$\Delta\rho_1(k_y, k_z, x) = \frac{2}{\pi}\left(\sqrt{2(E_x - V)} - \sqrt{2E_x}\right)$$

$$+ \frac{V''}{12k_x^3} + \frac{V'^2}{8k_k^5} + \ldots\Big);$$

$$E_x = \mathscr{E} - (k_y^2 + k_z^2)/2, \qquad k_x = \sqrt{k_m^2 - k_y^2 - k_z^2}. \tag{4.3}$$

*Otherwise, integrating up to $\mathscr{E}$ from below, we would be confronted with the inapplicability of the Born approximation to the low-energy particles with $E \lesssim V_{max}$, and to the bound particles in the case V < 0.

We find the total change of the density by integrating over dk_y, dk_z. We note that in polar coordinates q, φ in the plane of k_y, k_z

$$dk_y dk_z = q\,dq\,d\varphi, \qquad k_x = \sqrt{k_m^2 - q^2}, \quad q\,dq = k_x dk_x,$$
$$\Delta\rho_3(x) = (2\pi)^{-1}\int \Delta\rho_1(k_x,\ x)\,k_x dk_x, \tag{4.4}$$

where the index 1 marks the solution for the one-dimensional motion, and the index 3 marks the desired solution for the three-dimensional motion. The expression (4.4) is exact if one uses the exact expression for $\Delta\rho_1(k_x, x)$, since the separation of the variables is exact.*

When, however, we substitute in Eq. (4.4) the quasiclassical expression for $\Delta\rho_1$ according to Eqs. (3.3) and (4.3), we encounter the fact that the integration starts from small k_x, where these quasiclassical formulas cannot be applied, and for all the terms except the first the integrals diverge in the region of small k_x.

Let us divide the range of integration over k_x in Eq. (4.4) into two parts. For $k_x < K$ (K is some boundary momentum) we integrate the exact, not quasiclassical, $\Delta\rho_1$. Above K we use the quasiclassical expression (3.3) and (4.3). Thus we have

$$\Delta\rho_3(k_m,\ x) = \Delta\rho_3(K,\ x) + (2\pi)^{-1}\int_K^{k_m} \Delta\rho_1(k_x,\ x)\,k_x dk_x. \tag{4.5}$$

It is natural to make the assumption that in the limit $k_m \to \infty$ the value of $\Delta\rho_3$ satisfies the statistical formula (1.2) without corrections,

$$\Delta\rho_3(k_x,\ x) \to (3\pi^2)^{-1}\{(k_m^2 - 2V)^{3/2} - k_m^3\} = \Delta\rho_3^0(k_m,\ x), \tag{4.6}$$

i.e., that the corrections go to zero for $k_m \to \infty$.

Comparing Eqs. (4.5) and (4.6), we find that (4.6) is just the integral of the first term of the one-dimensional expression [the term corresponding to Eqs. (1.1) and (2.9)]

$$(k_m^2 - 2V)^{3/2} - k_m^3 = \int_{\sqrt{2V}}^{k_m} (k_x^2 - 2V)^{1/2} k_x dk_x - \int_0^{k_m} k_x^2 dk_x, \tag{4.7}$$

and consequently to each successive (i-th) correction term in Eq. (4.3) there correspond two terms in Eq. (4.5), whose sum goes to zero for $k_m \to \infty$. From this we have

$$\Delta\rho_{3i}(x) = \Delta\rho_{3i}(K,\ x) + (2\pi)^{-1}\int_K^{k_m} \Delta\rho_{1i}(k_x,\ x)\,k_x\,dk_x$$
$$= -(\pi/2)\int_{K_m}^{\infty} \Delta\rho_{1i}(k_x,\ x)\,k_x\,dk_x. \tag{4.8}$$

Thus in the three-dimensional case the principle of carrying over the summation from the region below k_m to that above k_m can be applied to the corrections, although it is not applicable to the main statistical term.*

*For $V < 0$, when there is a bound level corresponding to $k_x^2 < 0$, it is understood that the integral in Eq. (4.4) also includes the sum over the discrete levels.

*We note that if we expand the main statistical term in powers of V and regard the terms in V^2, V^3, ... as corrections, then the principle of transferring the summation can also be applied to them, and their signs are also opposite in the one-dimensional and three-dimensional cases.

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260