PHYSICAL REVIEW
LETTERS

VOLUME 14 8 MARCH 1965 NUMBER 10

PHASE TRANSITION IN THE HARTREE-FOCK ELECTRON GAS*

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(Received 9 February 1965)

The first two terms in the high-density expansion for the energy of a degenerate electron gas imbedded in a uniform background of positive charge are given correctly by the Hartree-Fock theory.[1] In this formulation, one neglects all correlations except those due to the Pauli principle, and thus the effective interaction, which acts only between particles of parallel spin, is purely attractive. The purpose of the present note is to point out that for moderately high densities—for which it is often assumed that the HF theory is a convenient starting point for the analysis of such a system—the electron gas as described by the HF theory undergoes a phase transition analogous to the familiar liquid-gas transition. The density at which this occurs is of order 10^{22}/cc and is not related to the melting of the Wigner lattice[2] which occurs at much lower densities.[3] Further, since we assume no polarization of the spins, this transition is not connected with the spin-density waves studied by Overhauser.[4] Mathematically speaking, the phase transition occurs because, as will be shown below, the particle density $n(\mu)$, when considered as a function of the chemical potential μ, has a finite discontinuity for a certain value μ_0 and this implies[5] the existence of a first-order phase transition.

In units in which all lengths are expressed in terms of the radius of the first Bohr orbit and all energies in Rydbergs, the single-particle energy of an electron of momentum $\vec{k}$ is given in the HF theory by

$$\epsilon(k) = k^2 - \frac{1}{\pi^2}\int d\vec{q}\,\frac{1}{(\vec{q}-\vec{k})^2+\lambda^2}\theta(\mu-\epsilon(\vec{q})), \qquad (1)$$

where, for generality, we have introduced a shielding parameter λ, and where θ is the step function which vanishes for negative values of its argument and is unity for positive ones. The relationship in Eq. (1) is, of course, well known, although customarily the θ function which appears under the integral is not present, but rather the domain of integration is restricted to be the interior of a sphere of radius k_0. The implied one-to-one relationship between the chemical potential μ and k_0 is always assumed although rarely spelled out in detail. For our purposes, we start with the "more basic" Eq. (1) and note that it is a nonlinear integral equation and that in general, for any given values for λ and μ, it may have more than one solution. Physically, this possibility of having a multiplicity of solutions of Eq. (1) offers no difficulty; and on reflection of the meaning and the origin of this equation, one concludes that we must select that solution for which the free energy (equivalently, the total energy) is a minimum. Because of this minimization criterion, it turns out that for a certain value of μ one must switch from one of these multiple solutions of Eq. (1) to another, and this change induces a discontinuity in $n(\mu)$ at this point, and thus[5] we have a phase transition.

To solve Eq. (1) we define a quantity $E(k, k_0)$ by the relation

$$E(k, k_0) = k^2 - \frac{1}{\pi^2}\int d\vec{q}\,\frac{1}{(\vec{q}-\vec{k})^2+\lambda^2}\theta(k_0-q), \qquad (2)$$

where k_0 is the parameter conventionally called the radius of Fermi sphere. On comparing Eqs. (1) and (2), it is clear that $E(k, k_0)$ will be a solution of Eq. (1) provided that[6]

$$\frac{\partial}{\partial k}E(k, k_0) > 0, \qquad (3)$$

and, in addition, that k_0 is determined by the relation

$$E(k_0, k_0) = \mu. \qquad (4)$$

Now it is easily confirmed by use of Eq. (2) that the condition in Eq. (3) is always satisfied, and Eq. (4) then tells us the value of the parameter k_0 for any given value of the chemical potential μ. In terms of the solution as expressed in Eqs. (2) and (4), the particle density as a function of μ becomes

$$n(\mu) = \frac{2}{(2\pi)^3}\int d\vec{k}\,\theta(\mu - \epsilon(\vec{k})) = \frac{1}{3\pi^2}k_0^3, \qquad (5)$$

where k_0 is to be thought of as a function of μ according to Eq. (4).

Let us now examine the possibility that Eq. (1) has more than one solution. First, we note that

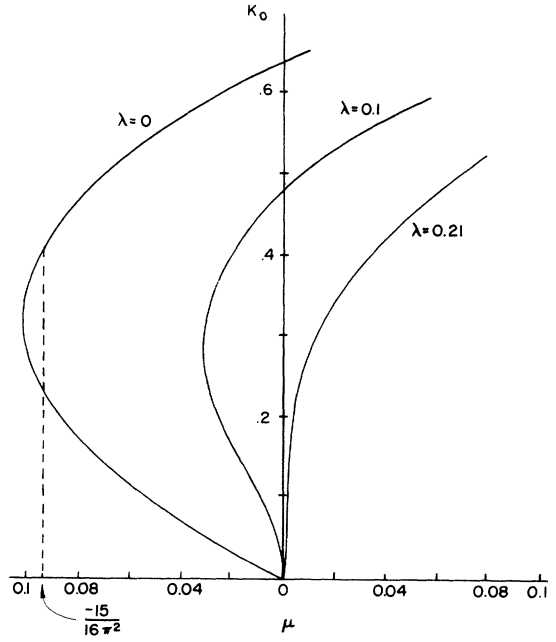

FIG. 1. Plot of k_0 as a function of $\mu[=E(k_0, k_0)]$ for various values of λ according to Eq. (4). For the case $\lambda = 0$, the solution which minimizes the free energy jumps at $\mu = -15/16\pi^2$ from the value $k_0 = 0$ to the upper curve, $k_0 = (1/\pi)[1 + (1+\mu\pi^2)^{1/2}]$.

for any negative value of μ, a solution of Eq. (1) is given by

$$\epsilon(k) = k^2, \quad \mu < 0; \qquad (6)$$

and according to the first equality in Eq. (5), $n(\mu)$ vanishes for such values of μ. The number of solutions of Eq. (1) of the form in Eq. (2) is clearly given by the number of values of k_0 which satisfy Eq. (4) for any given μ. In Fig. 1 we give a plot of k_0 as a function of $\mu[=E(k_0, k_0)]$ for several values of λ. For all values of λ larger than approximately 0.21, for any given value of μ there is a unique value for k_0 and, according to Eq. (5), a unique density. However, for values of λ less than 0.21, it is seen from Fig. 1 that for a certain range of values of μ there are three[7] values of k_0 which will satisfy Eq. (4) and, correspondingly, these are three solutions of Eq. (1). The minimization criterion noted above tells us to select that solution which minimizes the free energy F. In terms of the density in Eq. (5) the free energy F may be written

$$F(\mu) = -\int_{-\infty}^{\mu} n(\mu)d\mu = -\frac{1}{3\pi^2}\int_0^{\mu} k_0^3 d\mu,$$

and evaluating this for the three possible solutions enables one then to find the value of μ at which $n(\mu)$ has a discontinuity. For the case $\lambda = 0$, one finds easily in this way that for values of $\mu < -15/16\pi^2$, the correct solution corresponds to $k_0 = 0$, while to the right of this point it lies on the upper curve of Fig. 1 which is given by

$$k_0 = \frac{1}{\pi} + \left(\frac{1}{\pi^2} + \mu\right)^{1/2}.$$

Thus at the point $\mu = -15/16\pi^2$, the density jumps discontinuously from the value zero to the value $125/192\pi^5$, and this implies[5] that there is a phase transition in the electron gas at a density $\sim 10^{22}$/cc. In Fig. 2 we give a plot of the values of k_0 at which the phase transition occurs for various values of the shielding parameter λ. Perhaps most noteworthy, is the fact that the phase transition disappears for values of $\lambda \gtrsim 0.20$.

One of the questions that arises naturally in the light of the present result is this: what is the effect of including correlations in addition to those produced by the Pauli principle? Formulas for this correlation energy in the high-density limit have been obtained by Gell-Mann and Brueckner,[8] for low densities by Wigner,[9]

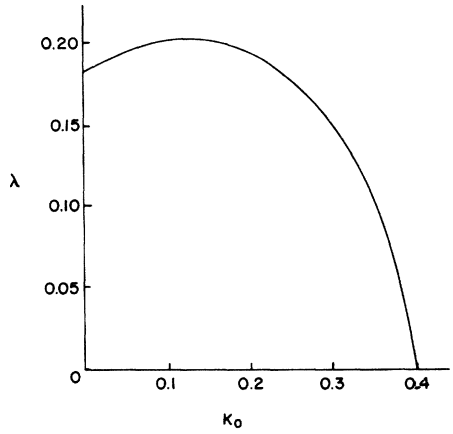

FIG. 2. Curve depicting the value of k_0 at which a phase transition occurs for various values of λ. The associated densities are given by Eqs. (4) and (5).

and there is also an intermediate-density formula given by Nozières and Pines.[10] In a report to be published elsewhere, it will be shown that the presently described phase transition is contained within all of these formulas at approximately the same density. This can be easily confirmed by noting that since the density fluctuations $\partial n/\partial \mu$ must be non-negative, it follows that the curve for the total energy as a function of density must always have positive curvature. And each of the above formulas has negative curvature for some range of densities, thus indicating at least the inapplicability of the formula for this region of densities. Further, the phase transition described here is also present if one includes lowest order temperature effects.

*Supported in part by U. S. Office of Aerospace Research, U. S. Air Force Grant No. AF-AFOSR 274-64.

[1]See, for example, R. Brout and C. Carruthers, Lectures on the Many-Electron Problem (Interscience Publishers, Inc., New York, 1963), Chap. 3.

[2]E. P. Wigner, Trans. Faraday Soc. 34, 678 (1938).

[3]F. De Wette, Phys. Rev. 135, A287 (1964).

[4]A. W. Overhauser, Phys. Rev. Letters 4, 415 (1960); and Phys. Rev. 128, 1437 (1962).

[5]See, for example, Kerson Huang, Statistical Mechanics (John Wiley & Sons, Inc., New York, 1963), p. 319.

[6]This condition is somewhat stronger than required but is sufficient for our purposes.

[7]Recall that, according to Eqs. (5) and (6), all negative values of μ may by associated with the solution of zero density.

[8]M. Gell-Mann and K. Brueckner, Phys. Rev. 106, 364 (1957).

[9]E. P. Wigner, Phys. Rev. 46, 1002 (1934).

[10]P. Nozières and D. Pines, Phys. Rev. 111, 442 (1958).

NEUTRON STARS*

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(Received 11 January 1965)

Several authors[1-5] have suggested that the recently discovered[5-7] extraterrestrial sources of x rays may be hot neutron stars. The plausibility of this suggestion, and in fact the likelihood that astronomers will ever be able to observe neutron stars by their x-ray emission, depend critically upon the cooling times of the hot stars. The main purposes of this note are (i) to present the results, and suggest the implications, of some approximate calculations for the neutrino cooling rates of neutron stars, and (ii) to point out that some current ideas regarding the constituents of neutron stars should be revised. Our description of the states of a neutron star and the reactions by which it cools differ from the work of previous authors[2,3,8] in that we include in an approximate way the effects of the strong interactions among all the hadrons (strongly interacting particles) present. The principal new results obtained (for densities not much greater than nuclear densities) are[9] (i) the existence of effective masses for all the hadrons, (ii) differential shifts in the threshold densities at which various kinds of particles are produced, and (iii) much faster cooling rates than previous workers have estimated. At densities greater than 10 times nuclear densities, unsolved matters of principle are of primary importance.[10] We have therefore attempted to phrase our initial questions in terms of quantities that can be defined independent of any specific model for the interaction among the particles that constitute a neutron star. Our practical results are, of course,