

# Stability of the Plane Wave Hartree-Fock Ground State

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The condition that the plane wave state is the lowest Hartree-Fock state of a large fermion system with repulsive interactions, is generally investigated and applied to the systems with  $\delta$ -type interactions, finite-range interactions, and long-range Coulomb interactions. It is found that for finite-range interactions the plane wave state is stable in both the high-density and low-density regions, but may become unstable in the intermediate-density region. The high-density stable region disappears for  $\delta$ -type interactions, while the low-density stable region vanishes for long-range Coulomb interactions. Especially for an electron gas, the critical value  $r_s$  is smaller than 4.5. A speculation concerning the transition of the true ground state is discussed.

## I. INTRODUCTION

LET us consider the ground state of a large fermion system with repulsive interactions. Self-evidently, a set of plane wave functions is a Hartree-Fock solution of the system. For this reason we usually start from the degenerate Fermi gas as the approximate ground state and calculate the correlation effects in a suitable way. However, the degenerate Fermi gas is not always the ground state of the Hartree-Fock equation: For example, electrons form a lattice at low density. In such a case the product of single-particle functions localized at each lattice point will give a lower energy expectation value than that of the degenerate Fermi gas state. In this paper we will discuss generally the condition that the degenerate Fermi gas state is the lowest Hartree-Fock solution and apply the condition to the systems with various interactions.

Several works have been done in this direction: Bloch<sup>1</sup> was the first who noticed the critical density below which electrons change to the ferromagnetic state because the exchange energy decrease overcompensates the kinetic energy increase. Recently, Overhauser<sup>2</sup> has found that in the one-dimensional fermion system the degenerate Fermi gas state is always unstable even for repulsive interactions. With respect to this remarkable fact, Kohn and Nettel<sup>3</sup> have pointed out that in the two- or more-dimensional case the situation is different and the degenerate Fermi gas remains the lowest Hartree-Fock state for sufficiently weak interactions. Wolff<sup>4</sup> also discussed this problem in connection with the magnetic susceptibility of an electron gas.

In this paper we will proceed as follows: We will consider the energy expectation value with respect to the Slater determinant composed of a set of single-particle functions. Of course, as a functional of single-

particle functions, the energy expectation value is stationary at the point where the single-particle functions are the Hartree-Fock solution. This Hartree-Fock state is stable or unstable according as the corresponding point is the minimum point or the maximum or saddle point. In the next section we will derive an eigenvalue equation which characterizes the local property around the point corresponding to the degenerate Fermi gas state. From Sec. III to Sec. V we will solve the eigenvalue equation for the systems with  $\delta$ -type interactions, finite-range interactions, and long-range Coulomb interactions, thereby we will find the density region where the degenerate Fermi gas state is stable. In Sec. VI some aspects of the true ground state will be discussed.

## II. STABILITY CONDITION

We will examine the behavior of the energy expectation value in the neighborhood of the degenerate Fermi gas state.

Let the plane-wave functions be  $\phi_i$  with momentum  $\mathbf{p}_i$  and spin in the  $u_i$  state:

$$\phi_i(\mathbf{r}, \sigma_z) = (e^{i\mathbf{p}_i \cdot \mathbf{r}} / \Omega^{1/2}) u_i(\sigma_z). \quad (1)$$

We will introduce the orthonormal single-particle functions  $\psi_i$  which are slightly different from the corresponding  $\phi_i$  by terms of the order of  $\epsilon$ :

$$\psi_i = [1 - \frac{1}{2}\epsilon^2(X_i, X_i)]\phi_i + \epsilon X_i + \epsilon^2 \eta_i + O(\epsilon^3), \quad (2)$$

with

$$(X_i, \phi_i) + (\phi_i, X_i) = 0, \quad (\eta_i, \phi_i) + (\phi_i, \eta_i) = 0. \quad (3)$$

$X_i$  may be expanded in a following form:

$$X_i(\mathbf{r}, \sigma_z) = \sum_{\lambda=0}^3 \sum_{\mathbf{p}_k} A^\lambda(\mathbf{p}_i, \mathbf{p}_k) (e^{i\mathbf{p}_k \cdot \mathbf{r}} / \Omega^{1/2}) \Gamma_\lambda u_i(\sigma_z), \quad (4)$$

with

$$\Gamma_0 = 1, \quad \Gamma_{1,2,3} = \sigma_x, \sigma_y, \sigma_z. \quad (5)$$

The orthogonality condition of  $\psi_i$  requires that

$$A^{\lambda*}(\mathbf{p}_i, \mathbf{p}_j) + A^\lambda(\mathbf{p}_j, \mathbf{p}_i) = 0, \quad (6)$$

and

$$(X_i, X_j) + (\eta_i, \phi_j) + (\phi_i, \eta_j) = 0, \quad \text{for } i \neq j. \quad (7)$$

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<sup>1</sup> F. Bloch, Z. Physik **57**, 549 (1929).

<sup>2</sup> A. W. Overhauser, Phys. Rev. Letters **4**, 462 (1960); J. des cloizeaux, J. phys. radium **20**, 606 (1959); **20**, 751 (1959).

<sup>3</sup> W. Kohn and S. J. Nettel, Phys. Rev. Letters **5**, 8 (1960).

<sup>4</sup> P. A. Wolff, Phys. Rev. **120**, 814 (1960).

Let us construct the Slater determinant from  $\psi_i$  ( $i=1, 2, \dots, N$ ) corresponding to the original degenerate Fermi gas state, and consider the energy expectation value

$$E[\psi] = \sum_{i=1}^N (\psi_i | p^2/2m | \psi_i) + \frac{1}{2} \sum_{i,j=1}^N \{ (\psi_i \psi_j | V | \psi_i \psi_j) - (\psi_i \psi_j | V | \psi_j \psi_i) \}. \quad (8)$$

$$E_2 = \sum_{\mathbf{q}} \sum_{\lambda=0}^3 E^\lambda(\mathbf{q}),$$

$$\begin{aligned} E^\lambda(\mathbf{q}) = & \sum_{|\mathbf{p}| < p_F} \{ \epsilon(\mathbf{p} + \mathbf{q}) - \epsilon(\mathbf{p}) \} [A^{\lambda*}(\mathbf{p}, \mathbf{p} + \mathbf{q}) A^\lambda(\mathbf{p}, \mathbf{p} + \mathbf{q}) + A^{\lambda*}(-\mathbf{p}, -\mathbf{p} - \mathbf{q}) A^\lambda(-\mathbf{p}, -\mathbf{p} - \mathbf{q})] \\ & - \sum_{|\mathbf{p}|, |\mathbf{p}'| < p_F} V(\mathbf{p} - \mathbf{p}') [A^{\lambda*}(\mathbf{p}, \mathbf{p} + \mathbf{q}) A^\lambda(\mathbf{p}', \mathbf{p}' + \mathbf{q}) + A^{\lambda*}(-\mathbf{p}, -\mathbf{p} - \mathbf{q}) A^\lambda(-\mathbf{p}', -\mathbf{p}' - \mathbf{q})] \\ & - \sum_{|\mathbf{p}|, |\mathbf{p}'| < p_F} V(\mathbf{p} + \mathbf{p}' + \mathbf{q}) [A^{\lambda*}(\mathbf{p}, \mathbf{p} + \mathbf{q}) A^{\lambda*}(-\mathbf{p}', -\mathbf{p}' - \mathbf{q}) + A^\lambda(\mathbf{p}, \mathbf{p} + \mathbf{q}) A^\lambda(-\mathbf{p}', -\mathbf{p}' - \mathbf{q})] \\ & + 2\delta_{\lambda,0} V(\mathbf{q}) \{ \sum_{|\mathbf{p}| < p_F} [A^{0*}(\mathbf{p}, \mathbf{p} + \mathbf{q}) + A^0(-\mathbf{p}, -\mathbf{p} - \mathbf{q})] \} \{ \sum_{|\mathbf{p}'| < p_F} [A^0(\mathbf{p}', \mathbf{p}' + \mathbf{q}) + A^{0*}(-\mathbf{p}', -\mathbf{p}' - \mathbf{q})] \}, \quad (11) \end{aligned}$$

where  $V(\mathbf{q})$  is the Fourier transform of the interaction potential

$$V(\mathbf{q}) = V(|\mathbf{q}|) = \int V(r) e^{i\mathbf{q} \cdot \mathbf{r}} d\mathbf{r} / \Omega, \quad (12)$$

$\epsilon(\mathbf{p})$  the Hartree-Fock single-particle energy

$$\epsilon(\mathbf{p}) = p^2/2m + NV(0) - \sum_{|\mathbf{p}'| < p_F} V(\mathbf{p} - \mathbf{p}'). \quad (13)$$

From the orthogonality condition (6) we can see easily that  $\mathbf{p}$  and  $\mathbf{p}'$  summation in (11) cancel each other when  $\mathbf{p} + \mathbf{q}$  or  $\mathbf{p}' + \mathbf{q}$  lies inside the Fermi sphere. Therefore, in (11) we can understand the  $\mathbf{p}$  or  $\mathbf{p}'$  summations to be performed for  $|\mathbf{p}| < p_F < |\mathbf{p} + \mathbf{q}|$  or  $|\mathbf{p}'| < p_F < |\mathbf{p}' + \mathbf{q}|$ .

Now from (9) we can see that the degenerate Fermi gas state is stable or unstable according as all the  $E^\lambda(\mathbf{q})$ 's are positive definite forms or not. It depends on the eigenvalues  $\omega$  of the secular equation for (11)

$$\begin{aligned} [\omega - \omega_p(\mathbf{q})] \psi^\lambda(\mathbf{p}) &= - \sum_{\mathbf{p}'} [V(\mathbf{p} - \mathbf{p}') \psi^\lambda(\mathbf{p}') + V(\mathbf{p} + \mathbf{p}' + \mathbf{q}) \psi^{\lambda*}(-\mathbf{p}')] \\ &\quad + 2\delta_{\lambda,0} V(\mathbf{q}) \sum_{\mathbf{p}'} [\psi^\lambda(\mathbf{p}') + \psi^{\lambda*}(-\mathbf{p}')], \quad (14) \\ \{\omega - \omega_p(\mathbf{q})\} \psi^{\lambda*}(-\mathbf{p}) &= - \sum_{\mathbf{p}'} [V(\mathbf{p} - \mathbf{p}') \psi^{\lambda*}(-\mathbf{p}') + V(\mathbf{p} + \mathbf{p}' + \mathbf{q}) \psi^\lambda(\mathbf{p}')] \\ &\quad + 2\delta_{\lambda,0} V(\mathbf{q}) \sum_{\mathbf{p}'} [\psi^{\lambda*}(-\mathbf{p}') + \psi^\lambda(\mathbf{p}')], \end{aligned}$$

where

$$\begin{aligned} \omega_p(\mathbf{q}) &= \epsilon(\mathbf{p} + \mathbf{q}) - \epsilon(\mathbf{p}) \\ &= (\mathbf{p} \cdot \mathbf{q} + \frac{1}{2} q^2) / m \\ &\quad + \sum_{\mathbf{p}'} [V(\mathbf{p} - \mathbf{p}') - V(\mathbf{p} + \mathbf{p}' + \mathbf{q})]. \quad (15) \end{aligned}$$

In (14) and (15)  $\mathbf{p}'$  is summed for  $|\mathbf{p}'| < p_F < |\mathbf{p}' + \mathbf{q}|$ . Equation (14) is similar to but not the same as the

$E[\psi]$  differs from the degenerate Fermi gas energy  $E[\phi]$  by terms of the order of  $\epsilon^2$ :

$$E[\psi] = E[\phi] + \epsilon^2 E_2 + O(\epsilon^3), \quad (9)$$

since it is stationary at the point where  $\psi$  is the Hartree-Fock solution.

Inserting (2) and (4) into (8), we can express  $E_2$  as the quadratic form of  $A^\lambda(\mathbf{p}_i, \mathbf{p}_k)$ :

equation of the hole-particle normal modes. The relation will be discussed in the Appendix.

There are two types of solutions due to the symmetric character of Eq. (14); one is symmetric,

$$\psi^\lambda(\mathbf{p}) = \psi^{\lambda*}(-\mathbf{p}); \quad (16)$$

the other antisymmetric,

$$\psi^\lambda(\mathbf{p}) = -\psi^{\lambda*}(-\mathbf{p}). \quad (17)$$

It is clear from the structure of Eq. (14) that for repulsive interactions the lowest eigenvalue appears in the symmetric solution for  $\lambda=1, 2, 3$ . In this case we have the eigenvalue equation

$$[\omega_k(\mathbf{q}) - \omega] \psi(\mathbf{k}) = \sum_{\mathbf{k}'} [V(\mathbf{k} - \mathbf{k}') + V(\mathbf{k} + \mathbf{k}')] \psi(\mathbf{k}'), \quad (18)$$

where we have used the variable  $\mathbf{k} = \mathbf{p} + \frac{1}{2}\mathbf{q}$  instead of  $\mathbf{p}$ , so that from (15)

$$\omega_k(\mathbf{q}) = \mathbf{k} \cdot \mathbf{q} / m + \sum_{\mathbf{k}'} [V(\mathbf{k} - \mathbf{k}') - V(\mathbf{k} + \mathbf{k}')], \quad (19)$$

and  $\mathbf{k}'$  summation should be performed for  $|\mathbf{k}' - \frac{1}{2}\mathbf{q}| < p_F < |\mathbf{k}' + \frac{1}{2}\mathbf{q}|$ . In the following,  $\mathbf{k}$  summation will be performed in this region unless otherwise stated.

Now our problem becomes to find the lowest eigenvalue  $\omega$  of Eq. (18). If it is positive, the degenerate Fermi gas state is stable. If negative, it is unstable.

### III. SYSTEMS WITH $\delta$ -TYPE POTENTIAL

As the first application of our condition (18) we take the simplest example, i.e., systems with  $\delta$ -type interactions.

Assuming  $V(\mathbf{k})$  to be constant in (18)

$$V(\mathbf{k}) = 4\pi e^2 / \Omega \mu^2. \quad (20)$$

We easily obtain the equation which determines the

eigenvalue  $\omega$ :

$$\frac{8\pi e^2}{\Omega\mu^2} \sum_{\mathbf{k}} \frac{1}{\omega_{\mathbf{k}} - \omega} = 1. \quad (21)$$

It is clear that this equation has a negative  $\omega$  solution only when

$$\frac{8\pi e^2}{\Omega\mu^2} \sum_{\mathbf{k}} \frac{1}{\omega_{\mathbf{k}}} = \frac{2p_F m e^2}{\pi\mu^2} J(q) > 1, \quad (22)$$

where

$$J(q) = \int_0^1 dz \int_{|a-b|}^{a+b} \frac{k^2 dk}{kqz} = \frac{1}{2} + \frac{4-q^2}{8q} \ln \left| \frac{2+q}{2-q} \right|, \quad (23)$$

with  $a = \{1 - \frac{1}{4}q^2(1-z^2)\}^{\frac{1}{2}}$ ,  $b = \frac{1}{2}qz$ .  $J(q)$  is a monotonically decreasing function with  $J(0)=1$ . Therefore, the degenerate Fermi gas remains the lowest Hartree-Fock state as long as

$$p_F < \pi\mu^2/2me^2, \quad (24)$$

and the instability sets in from the small  $q$  value.

#### IV. CASE OF FINITE RANGE FORCE

In this section we will investigate the stability condition for the finite-range interaction which is assumed as

$$V(\mathbf{k}) = 4\pi e^2/\Omega(k^2 + \mu^2). \quad (25)$$

For this potential we use the relation

$$V(\mathbf{k} \pm \mathbf{k}') = \frac{4\pi e^2}{\Omega} \frac{2\pi}{kk'} \sum_{l=0}^{\infty} (\mp 1)^l Q_l \left( \frac{k^2 + k'^2 + \mu^2}{2kk'} \right) \times \sum_m Y_{lm}(\theta, \phi) Y_{l-m}(\theta', \phi'), \quad (26)$$

where the  $Q_l$ 's are Legendre functions of the second kind,<sup>5</sup>

$$Q_0(x) = \frac{1}{2} \ln \left| \frac{x+1}{x-1} \right|, \quad Q_1(x) = \frac{x}{2} \ln \left| \frac{x+1}{x-1} \right| - 1 \cdots; \quad (27)$$

$\theta, \phi$  or  $\theta', \phi'$  denotes the direction of  $\mathbf{k}$  or  $\mathbf{k}'$  with respect to the  $\mathbf{q}$  direction as the  $z$  axis.

Introducing the expansion (26) into (18) and measuring  $\mathbf{k}, \mathbf{k}'$  in unit of the Fermi momentum  $p_F$ , we have

$$kqz\psi(k, z, \phi) = \frac{me^2}{\pi p_F} \int_0^{2\pi} d\phi' \int_0^1 dz' \int_{|a'-b'|}^{a'+b'} \frac{k'}{k} \times \sum_{l,m} Q_l \left( \frac{k^2 + k'^2 + \mu^2/p_F^2}{2kk'} \right) Y_{lm}(\theta, \phi) Y_{l-m}(\theta', \phi') \times \{ [1 + (-1)^l] \psi(k', z', \phi') - [1 - (-1)^l] \psi(k, z, \phi) \}, \quad (28)$$

<sup>5</sup> P. M. Morse and H. Feshbach, *Method of Theoretical Physics* (McGraw-Hill Book Company, Inc., New York, 1953), Part II, p. 1327.

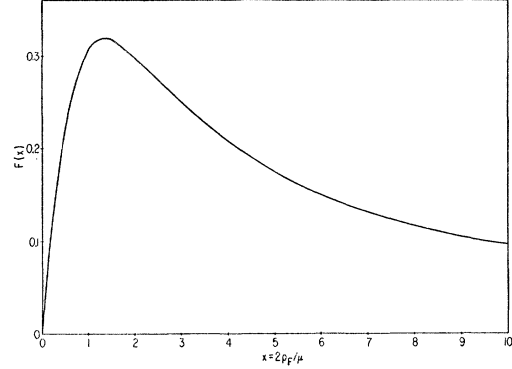


FIG. 1. The function  $F(x)$  is plotted against  $x = 2p_F/\mu$ .

with  $z = \cos\theta$ ,  $z' = \cos\theta'$ . In this equation we have already put  $\omega = 0$ , because we want to find the critical stability point, not the value  $\omega$  itself. Therefore, Eq. (28) should be regarded as the eigenvalue equation for  $(me^2/\pi p_F)_{\text{critical}}$ .

Generally, it is difficult to solve Eq. (28). However, we can find the exact solution for small  $q$  making use of the relation

$$\int_{|a-b|}^{a+b} dk f(k) = qz f(1) + O(q^3). \quad (29)$$

In this case it is easily seen that the eigenfunctions are

$$\psi(k, z, \phi) = Y_{lm}(\theta, \phi)/kqz, \quad l = \text{even}, \quad (30)$$

and the critical points are given by

$$(\pi p_F/me^2)_{\text{crit}} = Q_l(1 + \mu^2/2p_F^2) - Q_1(1 + \mu^2/2p_F^2), \quad (31)$$

with  $l = \text{even}$ .

Equation (31) does not give solutions for  $l \geq 2$ , because in these cases  $Q_l < Q_1$ . Inserting (27) into (31) with  $l=0$ , we have the stability condition

$$\pi\mu/2me^2 > F(2p_F/\mu), \quad (32)$$

with

$$F(x) = \frac{1}{x} - \frac{1}{x^3} \ln(1+x^2) \sim \begin{cases} x/2 & \text{for small } x, \\ 1/x & \text{for large } x. \end{cases} \quad (33)$$

Function  $F(x)$  is plotted in Fig. 1. We can see that for  $\pi\mu/2me^2 > 0.32$  the degenerate Fermi gas state is stable at all densities. For  $\pi\mu/2me^2 < 0.32$  the degenerate Fermi gas state is stable in both the high-density and low-density regions, but unstable in the intermediate-density region. The result may physically be interpreted as follows: At very low density where the mean particle distance is much larger than the force range, particles behave almost freely and the degenerate Fermi gas state is certainly stable. As the density increases, the repulsive forces become so effective that the particles tend to arrange themselves so as to keep away from each other, and the degenerate Fermi gas state may not be the lowest Hartree-Fock state. However, at very high density where the kinetic energy is dominant

and the potential energy becomes a small perturbation, the degenerate Fermi gas state is again stable.

In this connection it is interesting to see the limiting cases of condition (32). When we increase  $\mu$  and  $e$  keeping  $e/\mu$  constant, we have  $p_F < \pi\mu^2/2me^2$  using the asymptotic form for small  $x$  in (33). This is just the stability condition (24) for  $\delta$ -type interactions. In this case, the high-density stable region disappears. On the contrary, taking the limit  $\mu \rightarrow 0$  in order to investigate the case of long-range Coulomb interactions, we have the stability condition, using the asymptotic expression for large  $x$  in (33),

$$p_F > me^2/\pi \quad \text{or} \quad r_s < \pi/\alpha = 6.02, \quad (34)$$

where  $\alpha = (4/9\pi)^{1/2}$  and  $r_s = me^2/\alpha p_F$  as is usually defined in the electron gas theory. In this case there is no stable region at low density.

So far, we have discussed the stability condition taking small  $q$  only. The result is probably correct for the low-density stable region, as the example of the  $\delta$ -type interactions shows. However, this is not true for the high-density stable region as will be discussed in the next section.

## V. STABILITY OF AN ELECTRON GAS

In this section we will calculate the critical stability density of an electron gas using the variational expression for  $(r_s)_{\text{crit}}$  in the case of  $q$  values which are not small.

We have seen at the end of the last section that the degenerate electron gas state becomes unstable for  $r_s > \pi/\alpha$ , while Bloch<sup>1</sup> obtained the condition

$$r_s > 0.9\pi/\alpha. \quad (35)$$

There is a small discrepancy between (34) and (35). This seems rather puzzling, because our general treatment should give a smaller critical value than the Bloch value which was obtained by comparing energies in some restricted class of states. The reason is that our treatment in the last section was done only for small  $q$  values. Actually, the following calculation shows that the instability first takes place for  $q$  values which are not small.

Since it is difficult to solve Eq. (28) exactly for

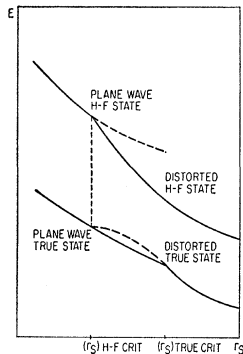


FIG. 2. A schematic ground-state energy diagram against  $r_s$  in the case of the true critical point being different from the Hartree-Fock critical point. The true states cross each other at both critical points.

general  $q$  values, we employ the following variational expression for the critical density:

$$\begin{aligned} (\alpha r_s/\pi)_{\text{crit}} &\leq N/(D_1 - D_2), \\ N &= \frac{1}{2\pi} \int |\psi(\mathbf{k})|^2 \mathbf{k} \cdot \mathbf{q} d\mathbf{k}, \\ D_1 &= \frac{1}{(2\pi)^2} \int \psi^*(\mathbf{k}) \left[ \frac{1}{|\mathbf{k} - \mathbf{k}'|^2} + \frac{1}{|\mathbf{k} + \mathbf{k}'|^2} \right] \psi(\mathbf{k}') d\mathbf{k} d\mathbf{k}', \\ D_2 &= \frac{1}{(2\pi)^2} \int |\psi(\mathbf{k})|^2 \left[ \frac{1}{|\mathbf{k} - \mathbf{k}'|^2} - \frac{1}{|\mathbf{k} + \mathbf{k}'|^2} \right] d\mathbf{k} d\mathbf{k}', \end{aligned} \quad (36)$$

with  $\mathbf{k}$  integrations to be done for

$$|\mathbf{k} - \frac{1}{2}\mathbf{q}| < 1 < |\mathbf{k} + \frac{1}{2}\mathbf{q}|.$$

Let us see first how the  $(r_s)_{\text{crit}}$  shifts from  $\pi/\alpha$  as the value  $q$  increases. For this purpose, we take the exact solution for small  $q$  [Eq. (30)] as the trial function  $\psi(\mathbf{k})$ :

$$\psi(\mathbf{k}) = 1/kqz, \quad (37)$$

and integrate (36) using the relation which includes the next-higher order terms of (29)

$$\begin{aligned} &\int_{|a-b|}^{a+b} dk f(k) \\ &= qz \left[ 1 - \frac{q^2}{8}(1-z^2) \frac{d}{dk} + \frac{q^2}{24} z^2 \frac{d^2}{dk^2} \right] f(k) \Big|_{k=1}. \end{aligned} \quad (38)$$

The result gives

$$(r_s)_{\text{crit}} \leq (1 - q^2/72 + \dots)(\pi/\alpha), \quad (39)$$

which indicates the decrease as was expected.

Since  $(r_s)_{\text{crit}}$  increases like  $q^4$  for very large  $q$ , we will now calculate (36) for  $q=2$  with the same trial function (37). In this case  $N$  and  $D_2$  can be integrated exactly, each giving

$$N = 1/2, \quad D_2 = \ln 2. \quad (40)$$

In order to perform the integration of  $D_1$ , we use the expansion (26) for the potential and calculate the terms corresponding to  $l=0, 2, 4$ . The result is

$$D_1 = 0.975 + 0.377 + 0.023 + \dots = 1.375. \quad (41)$$

This series converges very rapidly. Combining (40) and (41), we finally get

$$(r_s)_{\text{crit}} \leq 0.74\pi/\alpha = 4.5, \quad (42)$$

which is actually smaller than the Bloch value (35).

## VI. DISCUSSION

In this section we want to speculate about the transition of the true ground state and to comment concerning the nature of the transition.

So far, we have investigated the transition of the Hartree-Fock ground state. Then the serious question arises: Does the transition of the true ground state take place at the same critical density as that of the Hartree-Fock ground state? Especially for an electron gas, the result (42) of the last section shows that the critical point appears already in metallic densities, although it is difficult to compare the pure electron gas with the actual metals. There were arguments by Wigner<sup>6</sup> and by Pines<sup>7</sup> that the correlation effects induce the screening to the bare Coulomb forces and that the critical point will move to the much lower density. Their arguments may be true, but we also have the following speculation that the true transition seems to occur just at the Hartree-Fock critical density: Since the distorted Hartree-Fock ground state must be the same as the plane wave Hartree-Fock ground state at the critical point, it will go over to the same true state at the critical point after including the correlations. Therefore, if the true critical point occurs at the lower density, the true state corresponding to the distorted Hartree-Fock ground state must touch the true ground state at the Hartree-Fock critical point after crossing at the true critical point, as is shown in Fig. 2. Such a case seems rather improbable compared with the case of the common critical density as is shown in Fig. 3.

We can see that the spin aligned states are mixed in the distorted Hartree-Fock ground state: The expectation value of the total-spin  $z$  component  $\sum \sigma_z$  becomes positive if we choose

$$\sum_{\lambda=0}^3 A^\lambda \Gamma_\lambda = A(\sigma_x + i\sigma_y), \quad (43)$$

in the expansion (4) of  $\chi_i$ . However, it is difficult to see whether the distorted Hartree-Fock ground state represents the lattice structure or not, although in the electron gas case that the instability occurs first for not small  $q$  (probably for  $q=2$ ) is quite suggestive of a kind of periodicity of the order of the mean particle distance.

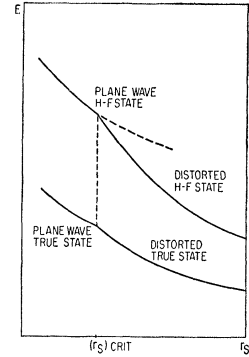
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<sup>6</sup> E. P. Wigner, Trans. Faraday Soc. **34**, 678 (1938).

<sup>7</sup> D. Pines, Phys. Rev. **92**, 626 (1953). Actually Dr. Langer has pointed out that the critical point moves to density zero if we take the static screening value  $\mu^2 = 4me^2 p_F / \pi$  in the stability condition (32).

FIG. 3. A schematic ground state energy diagram against  $r_s$  in the case of the critical point being common to Hartree-Fock and true states.



#### APPENDIX

The eigenvalue equation (14) is the same as the equation of the hole-particle normal mode<sup>8,9</sup> except the signs of  $\omega$ . The latter is connected to the quadratic form (11) in the following way.

Introducing the vector notation

$$\Psi_p(\lambda, \mathbf{q}) = \begin{pmatrix} A^\lambda(\mathbf{p}, \mathbf{p}+\mathbf{q}) \\ A^{\lambda*}(-\mathbf{p}, -\mathbf{p}-\mathbf{q}) \end{pmatrix}, \quad (44)$$

and  $\sigma_x, \sigma_y, \sigma_z$ : spin matrices operating on  $\Psi$ , we can rewrite (11) as

$$E^\lambda(\mathbf{q}) = \sum_{\mathbf{p}, \mathbf{p}'} \Psi_p^* [\omega_p \delta_{\mathbf{p}, \mathbf{p}'} + 2\delta_{\lambda,0} V(\mathbf{q})(1 + \sigma_x) - V(\mathbf{p}-\mathbf{p}') - V(\mathbf{p}+\mathbf{p}'+\mathbf{q})\sigma_x] \Psi_{p'}. \quad (45)$$

If we want to diagonalize this form with the metric  $\sigma_z$ :

$$E^\lambda(\mathbf{q}) = \sum_n \sum_p \omega^{(n)} \Psi_p^{(n)*} \sigma_z \Psi_p^{(n)}, \quad (46)$$

we have the usual equation of the pair normal mode:

$$[\omega^{(n)} \sigma_z - \omega_p] \Psi_p^{(n)} = \sum_{p'} [2\delta_{\lambda,0} V(\mathbf{q})(1 + \sigma_x) - V(\mathbf{p}-\mathbf{p}') - V(\mathbf{p}+\mathbf{p}'+\mathbf{q})\sigma_x] \Psi_{p'}^{(n)}. \quad (47)$$

$\Psi$  is connected to  $\Phi$  in reference 8 as

$$\Phi_p^{(n)} = \sigma_z \Psi_p^{(n)}. \quad (48)$$

Closer examination of instability relation (2.8) of reference 9 shows that the necessary condition for  $(\partial^2/\partial\lambda^2)E(\lambda)|_{\lambda=0}=0$  is that eigenvalue  $\omega$  be complex, since for complex  $\omega$  evaluation of  $\langle \Phi_0 [S, S^*] \Phi_0 \rangle$  shows that it is zero (simply because  $S$  and  $S^*$  belong to different eigenvalue  $\omega$  and  $\omega^*$  for complex  $\omega$ ). The statement made below Eq. (2.8) concerning the real eigenvalue  $\omega$  needs amendment, in general, and we should actually evaluate (2.8) to find out whether for given  $S$  the system is stable or not.

<sup>8</sup> K. Sawada and T. Soda, Phys. Rev. **123**, 1087 (1961).

<sup>9</sup> K. Sawada and N. Fukuda, Progr. Theoret. Phys. (Kyoto) **25**, 653 (1961).