Instability of Antiferromagnetic Screw-Type Structure of an Electron Gas*

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An analysis of antiferromagnetic screw-type structures in a three-dimensional electron gas is given, using a self-consistent field method. It is shown that a screw-type state appears to be always unstable. The expression for the susceptibility of an electron gas found by Wolff is also obtained with this method.

SEVERAL arguments have been published recently[1–4] to show that the screw-type structure of an electron gas proposed by Overhauser,[5] i.e. his "giant spin density wave," is unstable. The aim of this paper is to describe the results of an analysis of this problem using the self-consistent field (SCF) method and to point out that the susceptibility of an electron gas, obtained by Wolff[3] using the normal mode method in the random phase approximation, can also be obtained from the SCF method.

We take the following Hamiltonian:

$$H=H_1+H_2,$$
$$H_1=\sum_{\mathbf{k}}\epsilon(\mathbf{k})(a_{\mathbf{k}\uparrow}^{\dagger}a_{\mathbf{k}\uparrow}+a_{\mathbf{k}\downarrow}^{\dagger}a_{\mathbf{k}\downarrow})+\sum_{\mathbf{k}}h(2\mathbf{q})(a_{\mathbf{k}+2\mathbf{q}\uparrow}^{\dagger}a_{\mathbf{k}\uparrow}-a_{\mathbf{k}+2\mathbf{q}\downarrow}^{\dagger}a_{\mathbf{k}\downarrow}),\quad(1)$$
$$H_2=U\sum_i a_{i\uparrow}^{\dagger}a_{i\uparrow}a_{i\downarrow}^{\dagger}a_{i\downarrow},$$

with

$$a_{i\sigma}=N^{-\frac{1}{2}}\sum_{\mathbf{k}}\exp(i\mathbf{k}\cdot\mathbf{r}_i)a_{\mathbf{k}\sigma}.$$

Here $\mathbf{k}$ is the wave vector, i runs over the lattice points, and $h(2\mathbf{q})$ is an external field with sinusoidal space variation with a wave vector $2\mathbf{q}$. A delta-function potential (H_2) is assumed between electrons for simplicity. It has been used by Overhauser[5] and others[3,4] and the validity of this approximation is difficult to estimate. It is also assumed that the lattice has a Bravais structure. Anticipating a screw-type spin arrangement with a wave vector $2\mathbf{q}$, we make a transformation of the spin quantization axis for any lattice point $\mathbf{r}_i$:

$$a_{i\uparrow}=\alpha_i\cos(\theta_i/2)-\beta_i\sin(\theta_i/2),$$
$$a_{i\downarrow}=\alpha_i\sin(\theta_i/2)+\beta_i\cos(\theta_i/2),\quad(2)$$

where

$$\theta_i=2\mathbf{q}\cdot\mathbf{r}_i.$$

Next we replace H_2 by H_2', which is defined by

$$H_2'=U\sum_i(\alpha_i^{\dagger}\alpha_i\langle\beta_i^{\dagger}\beta_i\rangle+\beta_i^{\dagger}\beta_i\langle\alpha_i^{\dagger}\alpha_i\rangle-\langle\alpha_i^{\dagger}\alpha_i\rangle\langle\beta_i^{\dagger}\beta_i\rangle).\quad(3)$$

The resulting Hamiltonian is diagonalized by the canonical transformation

$$\alpha_i=N^{-\frac{1}{2}}\sum_{\mathbf{k}}\exp(i\mathbf{k}\cdot\mathbf{r}_i)\alpha_{\mathbf{k}},\quad\text{etc.},$$
$$\alpha_{\mathbf{k}}=A_{\mathbf{k}}\cos\varphi_{\mathbf{k}}+iB_{\mathbf{k}}\sin\varphi_{\mathbf{k}},\quad(4)$$
$$\beta_{\mathbf{k}}=iA_{\mathbf{k}}\sin\varphi_{\mathbf{k}}+B_{\mathbf{k}}\cos\varphi_{\mathbf{k}},$$

with

$$\tan2\varphi_{\mathbf{k}}=[\epsilon(\mathbf{k}+\mathbf{q})-\epsilon(\mathbf{k}-\mathbf{q})]/U\mu',$$

where

$$\mu'=\mu+(h/U),\quad\mu=\langle\alpha_i^{\dagger}\alpha_i\rangle-\langle\beta_i^{\dagger}\beta_i\rangle.\quad(5)$$

This gives

$$H=\sum_{\mathbf{k}}E_{\mathbf{k}}^{-}A_{\mathbf{k}}^{\dagger}A_{\mathbf{k}}+\sum_{\mathbf{k}}E_{\mathbf{k}}^{+}B_{\mathbf{k}}^{\dagger}B_{\mathbf{k}}+NU(n^2+\mu^2)/4,\quad(6)$$
$$E_{\mathbf{k}}^{\pm}=[\epsilon(\mathbf{k}+\mathbf{q})+\epsilon(\mathbf{k}-\mathbf{q})]/2\pm\{(U\mu'/2)^2+[\epsilon(\mathbf{k}+\mathbf{q})-\epsilon(\mathbf{k}-\mathbf{q})]^2/4\}^{\frac{1}{2}},\quad(7)$$

with

$$\mu=(U/N)\sum_{\mathbf{k}}[\mu'/(E_{\mathbf{k}}^{+}-E_{\mathbf{k}}^{-})][f(E_{\mathbf{k}}^{-})-f(E_{\mathbf{k}}^{+})],\quad(8)$$

where N is the number of lattice points, n is the number of electrons per atom, and $f(E)$ is the Fermi distribution function. Equation (8) is the SCF requirement.

When $h=0$ and if, for some $\mathbf{q}\neq0$, Eqs. (5) and (8) have a solution $\mu\neq0$, all the one-particle states of Eq. (6) have a screw-type spin orientation. If $\mu\neq0$ for $\mathbf{q}=0$, the spins of all the particles A point in the $+z$ direction, those of B in the $-z$ direction, and $E_{\mathbf{k}}^{+}-E_{\mathbf{k}}^{-}=U\mu$. This leads to a ferromagnetic state of the metal. If $\mu=0$ for any $\mathbf{q}$, the one-particle states are pairwise degenerate: $E_{\mathbf{k}+\mathbf{q}}^{-}=E_{\mathbf{k}-\mathbf{q}}^{+}=\epsilon(\mathbf{k})$ for $k_z>q$, $E_{\mathbf{k}+\mathbf{q}}^{-}=E_{\mathbf{k}-\mathbf{q}}^{-}=\epsilon(\mathbf{k})$ for $-q<k_z<q$, and $E_{\mathbf{k}-\mathbf{q}}^{-}=E_{\mathbf{k}+\mathbf{q}}^{+}=\epsilon(\mathbf{k})$ for $k_z<-q$ (k_z is the component of $\mathbf{k}$ along $\mathbf{q}$). This gives a paramagnetic state of the metal.

Taking free electrons, $\epsilon(\mathbf{k})=\hbar^2k^2/2m$ and $n=1$, our approach is equivalent to that of Overhauser.[5] For the free-electron case, it can be seen from Eq. (7) that the following three possibilities can be distinguished with regard to the relative position of the filled portion of the A and B bands:

$$\text{(I)}\quad x^2+2\nu\mu'<\epsilon^*,$$
$$\text{(II)}\quad x^2-2\nu\mu'<\epsilon^*<x^2+2\nu\mu',\quad(9)$$
$$\text{(III)}\quad\epsilon^*<x^2-2\nu\mu',$$

with

$$x=q/k_0,\quad\nu=U/4\epsilon_0,\quad\epsilon^*=E^*/\epsilon_0,$$

where $\hbar k_0$ and ϵ_0 are the Fermi momentum and the Fermi energy in a paramagnetic state, respectively, ν is

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proportional to the reciprocal of the effective density defined by Overhauser, and E^* is the Fermi energy in the screw-type state. The expression of $E_{\mathbf{k}}^{\pm}$ for free electrons is given by

$$E_{\mathbf{k}}^{\pm}/\epsilon_0=(k/k_0)^2+x^2\pm 2[\nu^2\mu'^2+x^2(k_z/k_0)^2]^{\frac{1}{2}}.$$

We have a maximum of $E_{\mathbf{k}}^{-}$ at the origin in the $\mathbf{k}$ space if $x^2>\nu\mu'$ and a minimum of $E_{\mathbf{k}}^{-}$ if $x^2<\nu\mu'$. Three cases are illustrated in Fig. 1.

For free electrons in three dimensions at $T=0$, the summations (integrations) over $\mathbf{k}$ in Eq. (8) and in the expression for the total energy, obtained from Eq. (6), can be carried out. For the three cases we find, respectively:

$$\text{(I)}\quad \epsilon_{\text{tot}}=\nu(1+\mu^2)+I_-(\zeta_+)+I_+(\zeta_-), \tag{10}$$

$$\mu=\mu'(3\nu/2)[G(\zeta_+)+2\zeta_--G(\zeta_-)], \tag{11}$$

$$1=\tfrac{3}{4}[F_-(\zeta_+)+F_+(\zeta_-)], \tag{12}$$

$$\text{(II)}\quad \epsilon_{\text{tot}}=\nu(1+\mu^2)+I_-(\zeta_+), \tag{13}$$

$$\mu=\mu'(3\nu/2)G(\zeta_+), \tag{14}$$

$$1=\tfrac{3}{4}F_-(\zeta_+), \tag{15}$$

$$\text{(III)}\quad \epsilon_{\text{tot}}=\nu(1+\mu^2)+I_-(\zeta_+)-I_-(\zeta_-), \tag{16}$$

$$\mu=\mu'(3\nu/2)[G(\zeta_+)-G(\zeta_-)], \tag{17}$$

$$1=\tfrac{3}{4}[F_-(\zeta_+)-F_-(\zeta_-)], \tag{18}$$

with

$$I_{\mp}(\zeta)=(\epsilon^*-x^4-4\nu^2\mu'^2)\zeta-2x^2\zeta^3-\tfrac{1}{5}\zeta^5 \pm\{[2x^2+\zeta^2+(\nu^2\mu'^2/4x^2)](\nu^2\mu'^2+x^2\zeta^2)^{\frac{1}{2}} +[2x-(\nu^2\mu'^2/2x^2)]\nu^2\mu'^2\sinh^{-1}(x\zeta/\nu\mu')\},$$

$$G(\zeta)=\zeta-(\zeta/4x^2)(\nu^2\mu'^2+x^2\zeta^2)^{\frac{1}{2}} +(1/2x)[\epsilon^*-x^2+(\nu^2\mu'^2/2x^2)]\sinh^{-1}(x\zeta/\nu\mu'),$$

$$F_{\pm}(\zeta)=(\epsilon^*-x^2)\zeta-\tfrac{1}{3}\zeta^3\mp[\zeta(\nu^2\mu'^2+x^2\zeta^2)^{\frac{1}{2}} +(\nu^2\mu'^2/x)\sinh^{-1}(x\zeta/\nu\mu')],$$

and

$$\zeta_{\pm}=\epsilon^*+x^2\pm 2(\nu^2\mu'^2+x^2\epsilon^*)^{\frac{1}{2}}.$$

Here ϵ_{tot} is the total energy per electron. Equations (11), (14), or (17) is the SCF requirement from Eq. (8), and Eqs. (12), (15), or (18), is an auxiliary equation to determine ϵ^* as a function of x and ν.

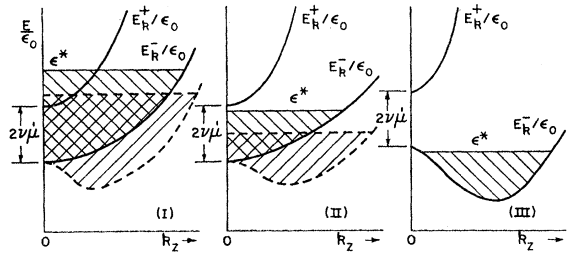

FIG. 1. Energy spectra of $E_{\mathbf{k}}^{\pm}$. The z axis is taken along the direction of $\mathbf{q}$. In the cases (I) and (II), the solid lines are for $x^2<\nu\mu'$ and the dashed lines for $x^2>\nu\mu'$.

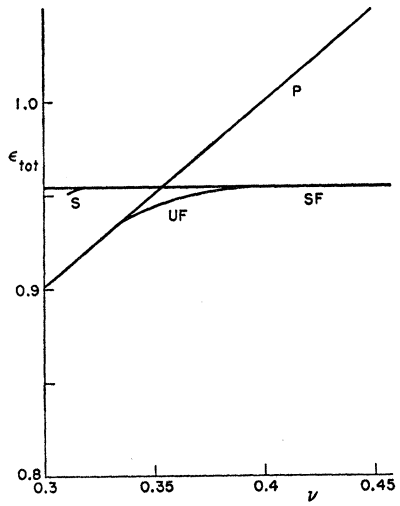

FIG. 2. Total energy vs ν. SF indicates the saturated ferromagnetic state, UF the unsaturated ferromagnetic state, P the paramagnetic state, and S the screw-type state.

Unfortunately, the complexity of the expressions in Eqs. (10)–(18) does not permit a complete analysis of all solutions. However, we can examine several particular cases. First of all, when $h=0$, as is well known, we have three stable solutions: ferromagnetic with only one band occupied (saturated) or with both bands partially occupied (unsaturated), and paramagnetic, depending on the magnitude of the parameter ν. Putting $x=0$ and $h=0$ in Eqs. (13)–(15), we have the saturated ferromagnetic state with $\mu=1$ and total energy $\epsilon_{\text{tot}}=3(2)^{\frac{2}{3}}/5$. In this solution the energy separation between the bottom of the B band and the filled position of the A band decreases as ν decreases and this energy separation vanishes at $\nu=2^{\frac{2}{3}}/4$. As ν decreases further, the unsaturated ferromagnetic state, obtained from Eqs. (10)–(12) with $x=0$, becomes stable. The quantity $N\mu$ is equal to difference between the number of electrons in the A and B bands; it decreases from the value N to 0 as ν decreases from $2^{\frac{2}{3}}/4$ to $\frac{1}{3}$. That is, the unsaturated ferromagnetic state becomes a paramagnetic state at $\nu=\frac{1}{3}$. The paramagnetic state is also obtained from Eqs. (10)–(18) with $\mu=0$ for any $\mathbf{q}$ value, and ϵ_{tot} of the paramagnetic state is $\frac{3}{5}+\nu$ (Fig. 2).

Secondly, when h/ϵ_0 and μ are very small, the expressions (11) and (17) both become, with the help of Eqs. (12) and (18), respectively,

$$\mu=\mu'(3\nu/2)F(x),$$

where

$$F(x)=1+[(1-x^2)/2x]\ln[(1+x)/|1-x|].$$

Since $\mu'=\mu+(h/U)$, we have

$$\mu=(h/\epsilon_0)\tfrac{3}{8}F(x)/[1-(3\nu/2)F(x)]. \tag{19}$$

The approximation (19) also holds for case (II), as follows from Eq. (14) with use of Eq. (15) after a careful expansion.

Equation (19) gives the same expression for the susceptibility as that derived by Wolff,[2] and we have also the same results for the stability of the paramagnetic state as those obtained by Kohn and Nettel,[1] Wolff,[2] and Brout.[3] That is, as long as $\nu<\frac{1}{3}$, the paramagnetic state is stable in such a sense that it does not go smoothly into a screw-type state with a very small μ.

Equation (19) can be obtained not only for a very small μ and $\hbar/\epsilon_0$ but also for a very small ν and finite μ' and x, because ν appears as a product $\nu\mu'$ in the functions G, $F_{\pm}$, and $\zeta_{\pm}$; and the expansion for a small μ', used in order to derive Eq. (19), was actually that for a small $\nu\mu'$. Therefore, we have no screw-type state for $\hbar=0$ in a limit of a very small ν.

Thirdly, we shall examine the stability of the saturated ferromagnetic state. This state belongs naturally to the case (II) ($\mu=1$ and $x=0$). If x is very small, an expansion of ϵ_{tot} with respect to x gives

$$\epsilon_{\text{tot}}\cong 3(2)^{\frac{2}{3}}/5+[1-(2^{\frac{2}{3}}/5\nu)]x^2. \tag{20}$$

At $\nu=2^{\frac{2}{3}}/5$, the saturated ferromagnetic state becomes unstable relative to a screw-type state with a very small x. The saturated ferromagnetic state, however, has already become unstable relative to the unsaturated ferromagnetic state for $\nu<2^{\frac{2}{3}}/4$ (Fig. 2).

Finally, for $\frac{1}{3}<\nu<2^{\frac{2}{3}}/4$, we can derive an expression similar to Eq. (20), but the coefficient of x^2 is positive for every value of ν in this interval. Therefore, a screw-type state with a very small x is never realized for this this range of ν values either.

We conclude that a screw-type state in a three-dimensional free electron gas appears never to become stable. A possibility for the existence of a screw-type state in a band model electron remains for a more complicated $\epsilon(\mathbf{k})$.

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