PHYSICAL REVIEW B VOLUME 7, NUMBER 5 1 MARCH 1973

Fluxon Coupling in Dual Thin Films

Max D. Sherrill
Physics Department, Clemson University, Clemson, South Carolina 29631
(Received 31 August 1972)

The coupling force for an isolated fluxon which extends through two thin films is calculated in the thin-film approximation. When the distance between centers of the fluxon in the two films is R, the force of attraction is $F_c = (\phi_0/\mu_0)\,[d_1d_2/(d_1\lambda_2^2 + d_2\lambda_1^2)]A_{d/\lambda^2}(R)$; $A_{d/\lambda^2}(R)$ is the vector potential describing the magnetic field distribution of a fluxon in a film for which d/λ^2 has the effective value $(d_1\lambda_2^2 + d_2\lambda_1^2)/\lambda_1^2\lambda_2^2$. The film thicknesses are d_1 and d_2, the penetration depths are λ_1 and λ_2, and ϕ_0 is the flux quantum. The result is obtained by using a simple superposition principle, and is valid when $d_1 \ll \lambda_1$, $d_2 \ll \lambda_2$, the fluxon core radii are much less than $2\lambda^2/d$, and the separation between the films is small compared to λ_1 or λ_2.

I. INTRODUCTION

Two planar superconducting films placed one upon the other and separated by a thin insulator act as a superconducting dc transformer.[1] The transformer action occurs because fluxons penetrate the two films and a current in one film induces fluxon motion in both so that a flux-flow voltage appears in both films. The operation of the transformer depends therefore upon the coupling force which can be exerted upon a fluxon in the secondary film because of a displacement of the fluxon in the primary film.

The objective of this paper is to calculate the coupling force for an isolated fluxon which extends through two thin superconducting films. We shall proceed by calculating the energy of the fluxon as a function of the distance between the centers of the fluxon in the two films and then obtain the coupling force as the negative derivative of the energy with respect to distance. All of the calculations will be valid when the film thicknesses d are much less than the penetration depths λ and when the coherence length ξ is must less than λ. This is the thin-film approximation which has been used by Pearl[2] to obtain the current and field distribution of an isolated fluxon in a single thin film and the force between two fluxons in a single thin film. The present calculation is an extension of Pearl's work which is well summarized in de Gennes.[3] The present calculation will apply only when the two films are very close together since it assumes that the vector potential is the same at both films. If the insulator thickness is less than the film thicknesses this approximation is less restrictive than the thin-film approximation.

We shall begin in Sec. II by calculating the familar result[2,3] for the force between two fluxons in a single film. This calculation will illustrate the methods used, and will develop some results which will be useful in the subsequent calculation of the coupling force in Sec. III.

II. FORCE BETWEEN FLUXONS IN A SINGLE FILM

The work done and consequently the increase in Hemholtz free energy upon placing a fluxon in a film may be written

$$F = \tfrac{1}{2}\int (\vec{J}\cdot\vec{A} + nmv^2)\,dV\ .$$

Here $\vec{J}$ is the current density, $\vec{A}$ is the vector potential, n is the number density of superelectrons, m is the electron mass, and v is the superelectron velocity. The integral is to be taken over the volume of the film excluding the fluxon core of radius ξ. The first term gives the magnetic field energy in the quasistationary approximation and the second term is the kinetic energy of the superelectrons. We neglect the condensation energy of the core which is small for $\xi \ll \lambda$.[3] With $\lambda^2 = m/\mu_0 ne^2$ and $\vec{J} = ne\vec{v}$ the Helmboltz free energy is

$$F = \tfrac{1}{2}\int (\vec{J}\cdot\vec{A} + \mu_0\lambda^2 J^2)\,dV\ . \tag{1}$$

For a fluxon $\vec{J}$ and $\vec{A}$ are related through the fluxoid quantum condition

$$\oint (\vec{A} + \mu_0\lambda^2\vec{J})\cdot d\vec{l} = \phi_0\ ,$$

where $\phi_0 = h/2e$ is the flux quantum. For circular symmetry there are only θ components for $\vec{A}$ and $\vec{J}$ so that

$$\vec{A} = [\,(\phi_0/2\pi r)\,\hat{\theta} - \mu_0\lambda^2\vec{J}\,]\ , \tag{2}$$

where $\hat{\theta}$ is a unit vector in the θ direction.

Suppose now that there are two fluxons whose centers are a distance R apart with one centered at $\vec{r}_1 = 0$ and the other at $\vec{r}_2 = 0$ so that $\vec{r}_1 - \vec{r}_2 = \vec{R}$. The total current density is in this case $\vec{J} = \vec{J}_1(\vec{r}_1) + J_2(\vec{r}_2)$. From Eq. (1) the increase in free energy is

$$F = \tfrac{1}{2}\int (\mu_0\lambda^2 J_1^2 + \mu_0\lambda^2 J_2^2 + \vec{J}_1\cdot\vec{A}_1 + \vec{J}_2\cdot\vec{A}_2)\,dV$$
$$+\tfrac{1}{2}\int (\vec{J}_1\cdot\vec{A}_2 + \vec{J}_2\cdot\vec{A}_1 + 2\mu_0\lambda^2\vec{J}_1\cdot\vec{J}_2)\,dV\ . \tag{3}$$

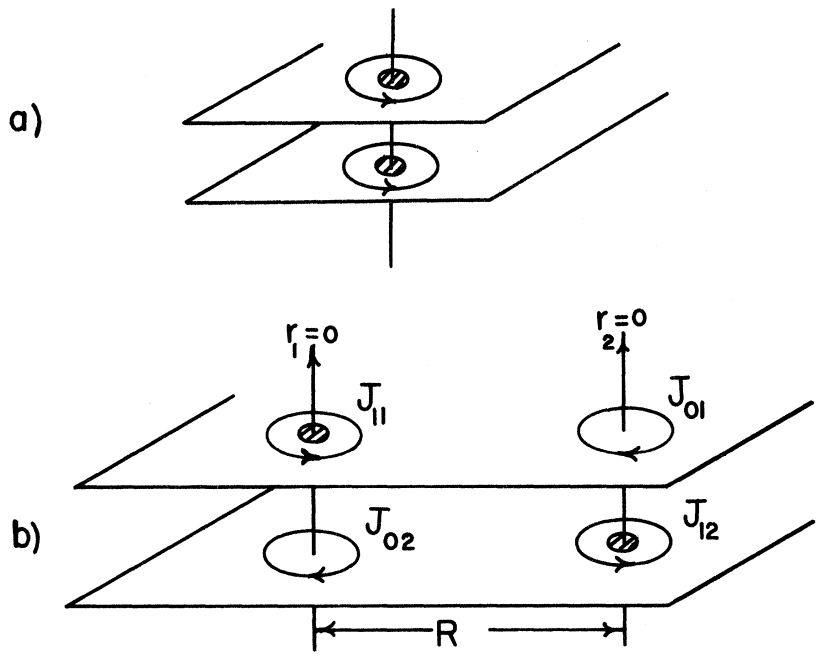

FIG. 1. Current distributions. In part (a) the fluxon is at the same place in both films. The core in film 2 lies beneath the core in film 1. The currents are in the same sense in both films. In (b) the cores in the two films are a distance R apart. The currents J_{01} and J_{02} are in the opposite sense to J_{11} and J_{12}. The currents J_{11} and J_{12} are larger than the currents in part (a).

The first term is twice the energy of an isolated fluxon and is independent of R. The second term is the interaction energy U_{12} and $-dU_{12}/dR$ will be the force between the fluxons. We note that the first two terms in U_{12} are equal so that we have

$$U_{12}=\int (\vec{J}_1\cdot\vec{A}_2+\mu_0\lambda^2\vec{J}_1\cdot\vec{J}_2)\,dV\,. \tag{4}$$

We may use Eq. (2) to express $\vec{A}_2$ as follows:

$$\vec{A}_2=\frac{\phi_0}{2\pi r_2}\,\hat{\theta}_2-\mu_0\lambda^2\vec{J}_2\,.$$

Substituting this expression for $\vec{A}_2$ into Eq. (4), we have

$$U_{12}=\frac{\phi_0}{2\pi}\int\frac{\hat{\theta}_2\cdot\vec{J}_1}{r_2}\,dV\,. \tag{5}$$

Since the current density is uniform through the thickness of the film d, we may write the integral as

$$U_{12}=\frac{\phi_0 d}{2\pi}\int_0^{2\pi}\int_\xi^\infty\frac{\hat{\theta}_2\cdot\vec{J}_1(\vec{r}_1)}{r_2}\,dr_1 d\theta_1$$
$$=\frac{\phi_0 d}{2\pi}\int_0^{2\pi}\int_\xi^\infty\frac{J_1(r_1)(r_1-R\cos\theta_1)r_1\,dr_1 d\theta_1}{r_1^2-2r_1R\cos\theta_1+R^2}\,. \tag{6}$$

The evaluation of this integral gives

$$U_{12}=\phi_0 d\int_R^\infty J_1(r_1)\,dr_1\,. \tag{7}$$

The repulsive force between the fluxons is $-dU_{12}/dR$, which is

$$F_{12}=-\frac{dU_{12}}{dR}=\phi_0 d\,J_1(R)\,. \tag{8}$$

This is the well-known result that the force on fluxon 2 is proportional to the current due to fluxon 1 at the core of fluxon 2.[3] $J_1(R)$ is given in Ref. 2.

III. COUPLING FORCE

Imagine first an isolated fluxon which extends through two planar-parallel films which are very close together as in Fig. 1(a). Since the films are thin ($d_1\ll\lambda_1$; $d_2\ll\lambda_2$) and the insulator thin, the vector potential and magnetic field are equal in the two films. Application of the fluxoid quantum condition Eq. (2) to each film gives

$$\vec{J}_1=\frac{1}{\mu_0\lambda_1^2}\left(\frac{\phi_0}{2\pi r}\,\hat{\theta}-\vec{A}\right),$$
$$\vec{J}_2=\frac{1}{\mu_0\lambda_2^2}\left(\frac{\phi_0}{2\pi r}\,\hat{\theta}-\vec{A}\right). \tag{9}$$

Using Pearl's[2] approach we express the total surface current density $d_1\vec{J}_1+d_2\vec{J}_2$ by using Eq. (9) and use $\nabla\times\vec{H}=(1/\mu_0)\nabla\times\nabla\times\vec{A}=-(1/\mu_0)\nabla^2\vec{A}=\vec{J}$ to obtain the differential equation

$$\nabla^2\vec{A}=-\mu_0(d_1\vec{J}_1+d_2\vec{J}_2)\delta(z)\,,$$
$$\nabla^2\vec{A}=-\frac{d_1\lambda_2^2+d_2\lambda_1^2}{\lambda_1^2\lambda_2^2}\left(\frac{\phi_0}{2\pi r}\,\hat{\theta}-\vec{A}\right)\delta(z)\,. \tag{10}$$

This is identical to Pearl's differential equation for the vector potential associated with a fluxon in a single film except that the initial factor in Eq. (10) has replaced the factor d/λ^2. We see that the dual film acts in this case as a single film with an effective value of d/λ^2 given by

$$\frac{d}{\lambda^2}=\frac{d_1\lambda_2^2+d_2\lambda_1^2}{\lambda_1^2\lambda_2^2}\ . \tag{11}$$

The solutions for $\vec{J}(r)$ and $\vec{A}(r)$, as given in Refs. 1 and 2, depend only upon the ratio rd/λ^2. We shall refer to these solutions as $\vec{A}_{d/\lambda^2}(r)$ and $\vec{J}_{d/\lambda^2}(r)$.

We wish to displace the center of the fluxon in film 2 relative to the center of the fluxon in film 1 and calculate the energy as a function of the separation R. By this we mean that the normal core in film 2 is displaced relative to the normal core in film 1. This displacement distorts the current and field distribution in both films so that the problem no longer has circular symmetry.

Figure 1(b) illustrates the situation when the fluxon is centered at different places in the two films. The fluxoid $\oint(\vec{A}+\mu_0\lambda^2\vec{J})\cdot d\vec{l}$ has the value ϕ_0 only when a normal region, the core, is included within the path of integration and the value zero otherwise. This means that if the fluxon is centered at $r_1=0$ in film 1 and at $r_2=0$ in film 2 $(\vec{r}_1-\vec{r}_2=\vec{R})$ then at $r_1=0$ in film 2 and at $r_2=0$ in film 1 there are screening currents. That is, at these locations the current densities are roughly opposite in direction to the vector potential.

To obtain the current distributions and the vector potential imagine that R is infinite. Under these circumstances the problem is now circularly symmetric about both $r_1=0$ and $r_2=0$. We will determine the current-density and vector-potential distribution for this circumstance and assume that the actual current and field distributions for finite R are a linear superposition of the solutions obtained for infinite R. This is in fact the same procedure used to obtain the force between two fluxons in a single film in Sec. II.

The situation in the dual film with R infinite is physically unrealistic and should be regarded as an aid to calculation only. Physically, the problem is of interest when R is of the order of a fluxon radius or smaller.

In Fig. 1(b) with R infinite we have the fluxon at $r_1=0$ in film 1 and at $r_2=0$ in film 2. The quantum conditions require that the integral $\oint(\vec{A}+\mu_0\lambda^2\vec{J})\cdot d\vec{l}$ is equal to ϕ_0 when the path of integration is about $r_1=0$ in film 1 or $r_2=0$ in film 2, whereas about $r_1=0$ in film 2 and about $r_2=0$ in film 1 it is equal to zero. Imagining now that R is infinite and using circular symmetry we can obtain the relationship between $\vec{J}$ and $\vec{A}$ in each case.

$$\vec{J}_{11}(r_1)=\frac{1}{\mu_0\lambda_1^2}\left(\frac{\phi_0}{2\pi r_1}\,\hat{\theta}_1-\vec{A}_1(r_1)\right)\ , \tag{12a}$$

$$\vec{J}_{02}(r_1)=-\frac{1}{\mu_0\lambda_2^2}A_1(r_1)\ , \tag{12b}$$

$$\vec{J}_{12}(r_2)=\frac{1}{\mu_0\lambda_2^2}\left(\frac{\phi_0}{2\pi r_2}\,\hat{\theta}-\vec{A}_2(r_2)\right)\ , \tag{12c}$$

$$\vec{J}_{01}(r_2)=-\frac{1}{\mu_0\lambda_1^2}\vec{A}_2(r_2)\ . \tag{12d}$$

Here the first subscript on the current densities refers to the quantum number which is zero or one and the second subscript refers to the film. $\vec{A}_1(r_1)$ describes the field distribution centered about $r_1=0$ and $\vec{A}_2(r_2)$ the distribution about $r_2=0$.

Proceeding as in the development of Eq. (10), the total surface current density centered about $r_1=0$ is $d_1\vec{J}_{11}(r_1)+d_2\vec{J}_{02}(r_1)$. Using Eqs. (12a) and (12b) we have

$$d_1\vec{J}_{11}(r_1)+d_2\vec{J}_{02}(r_1)=\frac{d}{\mu_0\lambda^2}\left(\frac{d_1\lambda^2}{d\lambda_1^2}\,\frac{\phi_0}{2\pi r_1}-\vec{A}_1(r_1)\right)\ , \tag{13}$$

where d/λ^2 is given by Eq. (11). As in the development of Eq. (10) this leads to

$$\nabla^2\vec{A}_1(r_1)=-\frac{d}{\lambda^2}\left(\frac{d_1\lambda^2}{d\lambda_1^2}\,\frac{\phi_0}{2\pi r_1}\,\hat{\theta}_1-\vec{A}_1(r_1)\right)\delta(r)\ .$$

This equation is identical to Eq. (10) except for the factor $d_1\lambda^2/d\lambda_1^2$. The solution for $\vec{A}_1(r_1)$ is therefore

$$\vec{A}_1(r_1)=\frac{d_1\lambda^2}{d\lambda_1^2}\,\vec{A}_{d/\lambda^2}(r_1)\ , \tag{14}$$

where as before $\vec{A}_{d/\lambda^2}$ is the vector potential of a fluxon in a single film with the value for d/λ^2 as given by Eq. (11).

Proceeding in the same way in the neighborhood of $r_2=0$, we obtain a similar expression for $\vec{A}_2(r_2)$,

$$\vec{A}_2(r_2)=\frac{d_2\lambda^2}{d\lambda_2^2}\,\vec{A}_{d/\lambda^2}(r_2)\ . \tag{15}$$

A fraction $d_1\lambda^2/d\lambda_1^2$ of the magnetic flux is centered about $r_1=0$ and a fraction $d_2\lambda^2/d\lambda_2^2$ about $r_2=0$. This is probably physically unrealistic but in any actual case where R is comparable with the fluxon size the superposition leads to a realistic distortion of the magnetic field distribution. The sum of $\vec{A}_1(r_1)$ and $\vec{A}_2(r_2)$ is equal to $\vec{A}_{d/\lambda^2}(r)$ when $r_1=r_2=r$ as it must be.

The total current density in film 1 is $\vec{J}_1=\vec{J}_{11}(r_1)+\vec{J}_{01}(r_2)$ and the total current density in film 2 is $\vec{J}_2=\vec{J}_{02}(r_1)+\vec{J}_{12}(r_2)$ and the total vector potential is $\vec{A}=\vec{A}_1(r_1)+\vec{A}_2(r_2)$. From Eqs. (12)

$$\begin{aligned} J_1&=\frac{1}{\mu_0\lambda_1^2}\left(\frac{\phi_0}{2\pi r_1}\,\hat{\theta}_1-\vec{A}\right)\ ,\\ J_2&=\frac{1}{\mu_0\lambda_2^2}\left(\frac{\phi_0}{2\pi r_2}\,\hat{\theta}_2-\vec{A}\right)\ , \end{aligned} \tag{16}$$

and the free energy is, from Eq. (1),

$$F=\tfrac{1}{2}\int_{V_1}(\vec{J}_1\cdot\vec{A}+\mu_0\lambda_1^2J_1^2)\,dV_1 +\tfrac{1}{2}\int_{V_2}(\vec{J}_2\cdot\vec{A}+\mu_0\lambda_2^2J_2^2)\,dV_2\ .$$

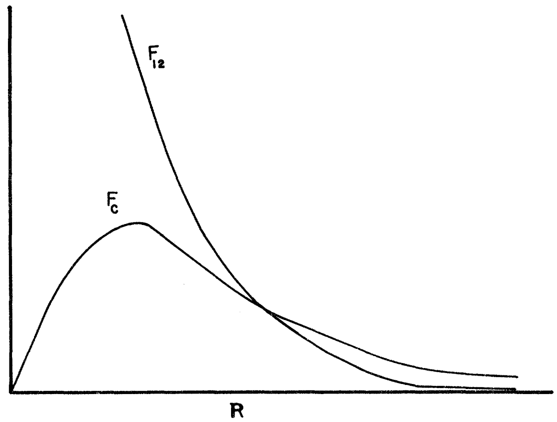

FIG. 2. Forces F_c and F_{12}. The fluxon coupling force F_c for two films each of thickness d is compared with the force between two fluxons F_{12} in a film of thickness $2d$.

From Eqs. (16) we note that

$$\vec{A}=\left(\frac{\phi_0}{2\pi r_1}\,\hat{\theta}_1-\mu_0\lambda_1^2\vec{J}_1\right)=\left(\frac{\phi_0}{2\pi r_2}\,\hat{\theta}_2-\mu_0\lambda_2^2\vec{J}_2\right),$$

so that

$$\vec{A}\cdot\vec{J}_1+\mu_0\lambda_1^2J_1^2=\frac{\phi_0}{2\pi r_1}\,\hat{\theta}_1\cdot\vec{J}_1\,,$$

$$\vec{A}\cdot\vec{J}_2+\mu_0\lambda_2^2J_2^2=\frac{\phi_0}{2\pi r_2}\,\hat{\theta}_2\cdot\vec{J}_2\,.$$

We have, therefore,

$$F=\frac{1}{2}\int_{V_1}\frac{\phi_0}{2\pi r_1}\,\hat{\theta}_1\cdot\vec{J}_1\,dV_1+\frac{1}{2}\int_{V_2}\frac{\phi_0}{2\pi r_2}\,\hat{\theta}_2\cdot\vec{J}_2\,dV_2\,.$$

Using the definitions of $\vec{J}_1$ and $\vec{J}_2$ and Eqs. (12), we have

$$F=\frac{\phi_0}{4\pi\mu_0\lambda_1^2}\int_{V_1}\left(\frac{\phi_0}{2\pi r_1^2}-\frac{1}{r}\,\hat{\theta}_1\cdot\vec{A}_1(r_1)-\frac{1}{r_1}\,\hat{\theta}_1\cdot\vec{A}_2(r_2)\right)dV_1$$
$$+\frac{\phi_0}{4\pi\mu_0\lambda_2^2}\int_{V_2}\left(\frac{\phi_0}{2\pi r_2^2}-\frac{1}{r_2}\,\hat{\theta}_2\cdot\vec{A}_1(r_1)-\frac{1}{r_2}\,\hat{\theta}_2\cdot\vec{A}_2(r_2)\right)dV_2.\qquad(17)$$

Again F may be expressed as a part F_0 which is independent of R and a part U_{12} which depends upon R. The terms in Eq. (17) which belong to U_{12} are those which depend upon both r_1 and r_2,

$$U_{12}=-\frac{\phi_0}{4\pi\mu_0\lambda_1^2}\int_{V_1}\frac{1}{r_1}\,\hat{\theta}_1\cdot\vec{A}_2(r_2)\,dV_1$$
$$-\frac{\phi_0}{4\pi\mu_0\lambda_2^2}\int_{V_2}\frac{1}{r_2}\,\hat{\theta}_2\cdot\vec{A}_1(r_1)\,dV_2\,.\qquad(18)$$

Both integrals are of the same form as the integral in Eq. (5). They differ only in that $\vec{A}_1$ and $\vec{A}_2$ appear in the place of $\vec{J}_1$. Evaluating the integrals as before, we have

$$U_{12}=-\frac{\phi_0 d_1}{2\mu_0\lambda_1^2}\int_R^\infty A_2(r_2)\,dr_2-\frac{\phi_0 d_2}{2\mu_0\lambda_2^2}\int_R^\infty A_1(r_1)\,dr_1\,.$$

The force of attraction is then given by $-dU_{12}/dR$:

$$F_c=-\frac{\phi_0 d_1}{2\mu_0\lambda_1^2}A_2(R)-\frac{\phi_0 d_2}{2\mu_0\lambda_2^2}A_1(R)\,.\qquad(19)$$

Using the expressions for $\vec{A}_1(r_1)$ and $\vec{A}_2(r_2)$ in Eqs. (14) and (15), we have

$$F_c=-\frac{\phi_0}{\mu_0}\,\frac{d_1d_2}{d_1\lambda_2^2+d_2\lambda_1^2}\,A_{d/\lambda^2}(R)\,.\qquad(20)$$

The equation says that the coupling force is attractive and depends upon separation in the same way that $A_{d/\lambda^2}(R)$ depends upon distance. $\vec{A}_{d/\lambda^2}(r)$ is of course the vector potential in the dual film when the primary and secondary fluxons are located at the same place. The result for the coupling force F_c looks formally like the repulsive force F_{12} between two fluxons in a single film except that the vector potential has replaced the current density $J(R)$. Their dependence upon R is, however, quite different as one can see immediately by considering the relationship between $\vec{J}$ and $\vec{A}$ as given in Eq. (2). This is shown in Fig. 2.

The force between two fluxons in a single film is proportional to $1/R$ for very small separations ($R\ll\lambda^2/d$) and proportional to $1/R^2$ when $R\gg\lambda^2/d$. The coupling force F_c must go to zero at least as fast as R for small separations since a vector potential which goes to zero less rapidly than r gives an infinite magnetic field intensity at the origin. At infinite distance the vector potential and therefore F_c must be proportional to $1/r$ because the fluxon contains a fixed amount of flux so $2\pi rA$ must equal ϕ_0 when r is infinite. These considerations guarantee that F_c will have a maximum value. This maximum in F_c and $\vec{A}(r)$ occurs at approximately $r=2\lambda^2/d^2$ and about half the flux of the fluxon, $\frac{1}{2}\phi_0$, is enclosed within this radius.

If we assume that the maximum coupling force occurs at $R=2\lambda^2/d$ and that half the flux is enclosed within this radius we can compare F_c and F_{12} at this distance. This will compare the force between two fluxons which extend through the two films and are a distance $2\lambda^2/d$ apart with the coupling force for a fluxon centered a distance $2\lambda^2/d$ apart in films 1 and 2. Using Eqs. (2) and (20) the maximum coupling force is approximately

$$F_c(R=2\lambda^2/d)\cong-\frac{\phi_0^2d_1d_2}{8\pi\mu_0\lambda_1^2\lambda_2^2}\,.\qquad(21)$$

Using Eq. (8) we find that for $d_1=d_2$ and $\lambda_1=\lambda_2$ this force is one-half F_{12} at $R=2\lambda^2/d$. This should not be taken as a comparison between the driving force and the coupling force in a dc transformer because F_{12} is not the driving force on the fluxon in the primary.

IV. CONCLUSION

The coupling force for an isolated fluxon in a dual-film system [Eq. (20)] is not identical with the coupling force on a fluxon in a superconducting dc transformer. The force F_c is, however, responsible for the operation of the transformer and probably represents the maximum coupling which can exist in a transformer. In the transformer the fluxons are not isolated and overlap of their current and field distributions serves to decrease the coupling. The transformer coupling is destroyed by perpendicular magnetic fields close to the critical field which may be only about 10 G (10^{-3} T). When there is no applied magnetic field and when the thin-film approximation ($d < \lambda$) is valid Eq. (20) may represent the transformer coupling reasonably well. For type-I films such as tin, the approximations should be reasonably accurate for film thicknesses up to about 10^{-7} m (1000 Å) and somewhat better for alloy films.

The film-thickness dependence of the coupling force predicted by Eqs. (20) and (21) agrees qualitatively with experiment. With the secondary thickness fixed the transformer coupling parameter (the ratio of secondary voltage to primary voltage) decreases with decreasing primary film thickness.[4] Since the coupling parameter is not simply related to the coupling force it is impossible to make a quantitative comparison between the calculation and these experiments.

ACKNOWLEDGMENTS

I have profited by discussions with J. R. Manson, M. J. Skove, and other associates during the course of this work.

[1]I. Giaever, Phys. Rev. Letters 15, 825 (1965); I. Giaever, Phys. Rev. Letters 16, 460 (1966); P. E. Cladis, Phys. Rev. Letters 21, 1238 (1968); P. E. Cladis, R. D. Parks, and J. M. Daniels, Phys. Rev. Letters 21, 1521 (1968).

[2]J. Pearl, Appl. Phys. Letters 16, 50 (1966); J. Pearl, *Proceedings of the Ninth International Conference on Low Temperature Physics* (Plenum, New York, 1965), Part A, p. 566.

[3]P. G. De Gennes, *Superconductivity of Metals and Alloys* (Benjamin, New York, 1966).

[4]M. D. Sherrill, Phys. Letters 24A, 312 (1967).

PHYSICAL REVIEW B VOLUME 7, NUMBER 5 1 MARCH 1973

Inhomogeneous Electron Gas*

A. K. Rajagopal and J. Callaway
Department of Physics and Astronomy, Louisiana State University, Baton Rouge, Louisiana 70803
(Received 17 May 1972)

This work is a generalization of the Hohenberg–Kohn–Sham theory of the inhomogeneous electron gas, with emphasis on spin effects. An argument based on quantum electrodynamics is used to express the ground-state energy of a system of interacting electrons as a functional of the current density. Expressions are derived for coefficients appearing in an expansion of the correlation functional in terms of the linear-response functions of the homogeneous system, for a gas of almost constant four-current density. The current density contains a spin-dependent term which leads, in the nonrelativistic limit, to a local potential which is also spin dependent. This potential is applied to the problems of spin splitting of energy bands in ferromagnets and spin-density-wave antiferromagnets. The relations between the present approach, that of Slater, and the collective electron theory of ferromagnetism of Stoner are described.

I. INTRODUCTION

Hohenberg and Kohn[1] (HK) and subsequently Kohn and Sham (KS)[2,3] developed a theory of the ground state of an interacting electron gas in the presence of an external potential $V(r)$. The essential concept of their treatment is that the energy is a universal functional of the density of the system $n(r)$ plus a linear functional of the potential $V(r)$. The functional of density $F[n]$ applies to all electronic systems in their ground state regardless of the specific form of the external potential $V(r)$.

The approach of HK does not include spin explicitly and therefore is not immediately useful in problems in which an external magnetic field is involved or in which magnetic order is present. This work presents a generalization of the treatment of