ambiguously distinguish whether the threefold or the onefold defect lies lower in energy. However, we consider our calculation to be an improvement upon earlier arguments based solely on electronic energies, which suggested that the threefold site would be distinctly lower.[9] In summary, we wish to emphasize the importance of using defect electron levels, and including repulsive interatomic terms, in estimating defect energies.

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Mean-Field Theory of Ferromagnetic Superconductors

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We present here a new mean-field theory of ferromagnetic superconductors in an external magnetic field. Simple models for the pure superconductor and the pure ferromagnet are chosen and the theory is considered in more detail. Phenomena predicted include both the destruction of superconductivity by the ferromagnetic order and the coexistence of ferromagnetism and superconductivity, as well as the magnetic field dependence of zero-temperature magnetization. Results obtained are in qualitative agreement with the experiments.

Considerable interest in the relationship between superconductivity and magnetism has been generated by the recent discoveries of magnetic transitions in superconducting alloys.[1-3] Destruction of superconductivity at the onset of long-range magnetic order raised many questions. The fundamental question of the coexistence of long-range magnetic order and superconductivity has been reopened, creating a stream of new experimental data.[4] Alloys analyzed were of the forms $M\mathrm{Rh}_4\mathrm{B}_4$,[1] $M_x\mathrm{Mo}_6\mathrm{Se}_8$,[2] and $M_x\mathrm{Mo}_6\mathrm{S}_8$, where M is a rare-earth element.[3] In $\mathrm{ErRh}_4\mathrm{B}_4$, for example, two transitions are observed[1]: At $T_{c1} \approx 8.7$°K the compound becomes superconducting, and then at a lower temperature $T_{c2} \approx 0.9°K$ it becomes ferromagnetic[5] while superconductivity is destroyed.

The new experiments present a challenging problem to the theorists. Existence of a regular lattice of rare-earth (RE) magnetic moments appears to be important. Therefore, microscopic theories, which consider a superconductor with magnetic impurities, like the Gor'kov-Rusinov[6] theory, may lead to inappropriate conclusions.[7] As a result, notable activity has been produced among theorists. Some of the on-going theoretical work is directed towards the microscopic theory of ferromagnetic superconductors (FS's). The problem, however, lies in the internal mathematical complexity of such a theory. Therefore, one may need a simple theory which provides the basic understanding and intuition necessary for developing a more detailed theory. This is the main reason we turned our attention to the mean-field theory.

Electronic structure calculations for some $M\mathrm{Rh}_4\mathrm{B}_4$ compounds[8] indicate that Rh $4d$ electrons are responsible for the superconductivity in these materials. They further indicate that RE localized magnetic moments, due to RE $4f$ electrons, are magnetically coupled via exchange interaction with RE $5d$ electrons. On the other hand, RE $4f$ electrons are weakly coupled to Rh $4d$ electrons. Therefore we will describe the FS as a coupled system of an ordinary superconductor (due to Rh) and the ferromagnetic lattice (due to RE). We will introduce coupling in a mean-field fashion, via screening effects, as described below.[9]

If we consider a completely decoupled system, then magnetizations[10] H_s and H_f, of the superconductor and ferromagnet, respectively, are given independently as

$$H_s = h_s(H_{\mathrm{ext}}, T) \tag{1}$$

and

$$H_f = h_f(H_{\mathrm{ext}}, T), \tag{2}$$

where H_{ext} is the external field, T is the temperature, and h_s and h_f are functions of these two variables. However, when there is a coupling, functions h_s and h_f must be modified. The simplest way to account for the coupling is via the screening of the external field: The superconductor sees the field $H_{\mathrm{ext},s}$, which is an external field screened by the ferromagnet, while, conversely, the ferromagnet sees the field $H_{\mathrm{ext},f}$, which is an external field screened by the superconductor.

Therefore [cf. Eqs. (1) and (2)],

$$H_s = h_s(H_{\mathrm{ext},f}, T), \quad H_f = h_f(H_{\mathrm{ext},s}, T), \tag{3}$$

where[11]

$$H_{\mathrm{ext},s} = H_{\mathrm{ext}} + H_f \tag{4}$$

and

$$H_{\mathrm{ext},f} = H_{\mathrm{ext}} + H_s. \tag{5}$$

Self-consistency requires Eq. (3) to be solved simultaneously for $H_s(H_{\mathrm{ext}}, T)$ and $H_f(H_{\mathrm{ext}}, T)$, by assuming that h_s and h_f are known functions, derived (or "given") for the superconductor and ferromagnet decoupled. The solution (or solutions) determine the total magnetization $M(H_{\mathrm{ext}}, T)$ of the FS as

$$M(H_{\mathrm{ext}}, T) = H_s(H_{\mathrm{ext}}, T) + H_f(H_{\mathrm{ext}}, T). \tag{6}$$

Our intention here is to present some qualitative predictions of the theory. For that purpose we consider simple model functions for h_s and h_f.[9] For the magnetization h_s of the pure superconductor we choose

$$h_s = \begin{cases} -H_{\mathrm{ext}}, & |H_{\mathrm{ext}}| \le h_1(T) \\ \mathrm{sgn}(H_{\mathrm{ext}})(\alpha h + \beta h^2)^{1/2} - H_{\mathrm{ext}}, & h_1(T) \le |H_{\mathrm{ext}}| \le h_2(T) \\ 0, & |H_{\mathrm{ext}}| \ge h_2(T) \end{cases} \tag{7}$$

where

$$h \equiv \frac{|H_{\mathrm{ext}}| - h_1(T)}{h_2(T) - h_1(T)}. \tag{8}$$

The lower critical field $h_1(T)$ and the upper critical field $h_2(T)$ are chosen as

$$h_{1,2}(T) = \begin{cases} h_{1,2}^0[1 - (T/T_s)^2], & T \le T_s \\ 0, & T \ge T_s \end{cases} \tag{9}$$

where T_s is the critical temperature for the pure superconductor. Constants α and β in Eq. (7) are chosen in such a way that h_s is smooth at $h = 1$. For the ferromagnetic system we choose a simple molecular-field model in which the magnetization h_f is implicitly given by

$$h_f = m_0 \tanh[(T_f/m_0 T)(H_{\mathrm{ext}} + h_f)], \tag{10}$$

where T_f is the ordering temperature for the ferromagnet and m_0 is its saturation magnetization. For simplicity we have assumed in Eq. (10) that the molecular field is the same as h_f.[12] There are five parameters involved in the model. However, by normalizing all fields to m_0 and all temperatures to T_s we need choose only three parameters: h_1^0, h_2^0, and T_f. The interplay of curves $h_{1,2}(T)$ and $h_f(0,T)$ determines the behavior of the FS. Accordingly, we can distinguish six typical cases (although some more peculiar cases may occur) in the model. Corresponding phase diagrams, obtained numerically, are presented in Fig. 1.

A large variety of phenomena can be observed in Fig. 1. However, we will analyze here only the phase diagram shown in Fig. 1(b). This case, $T_f < T_s$ and $h_1^0 < m_0 < h_2^0$, seems to resemble the experimental situation in $ErRh_4B_4$ most closely.[9] We first observe that there is a temperature T_{c2} below which superconductivity is destroyed and ferromagnetism occurs. T_{c2} is below the ordering temperature T_f for the pure ferromagnet. This is in agreement with the experimental observations.[1] Further analysis of the phase diagram shows that there are four phases present. First there is the normal phase $[M=h_f(H_{ext},T)$; $H_s=0]$ denoted n in the figure. In this region the FS behaves just as a pure ferromagnet would. Hence, one should be able to extract information about the ferromagnetic system (e.g., m_0, T_f) from the high-temperature field measurements (e.g., susceptibility). Three more phases can be observed: intermediate superconducting $[-H_{ext} < M < h_f(H_{ext},T)]$, intermediate superconducting ferromagnetic $[h_f(0,T) > M > 0 = H_{ext}]$, and pure superconducting $(M = -H_{ext};\ H_f = 0)$, denoted II, IIf, and I, respectively. Furthermore, there are regions in which unstable phases may occur. Thus there is a region, denoted I′, in phase I in which an unstable phase II occurs. There is an equivalent region, denoted II′, in phase II in which an unstable phase I occurs. Finally, in phase IIf there is a region, which we denote II′f, of unstable phase I. Corresponding discontinuous phase transitions are denoted by a heavy line in the figure. Dotted lines separate regions where unstable phases appear. Similarly, continuous transitions are denoted by the broken lines. It

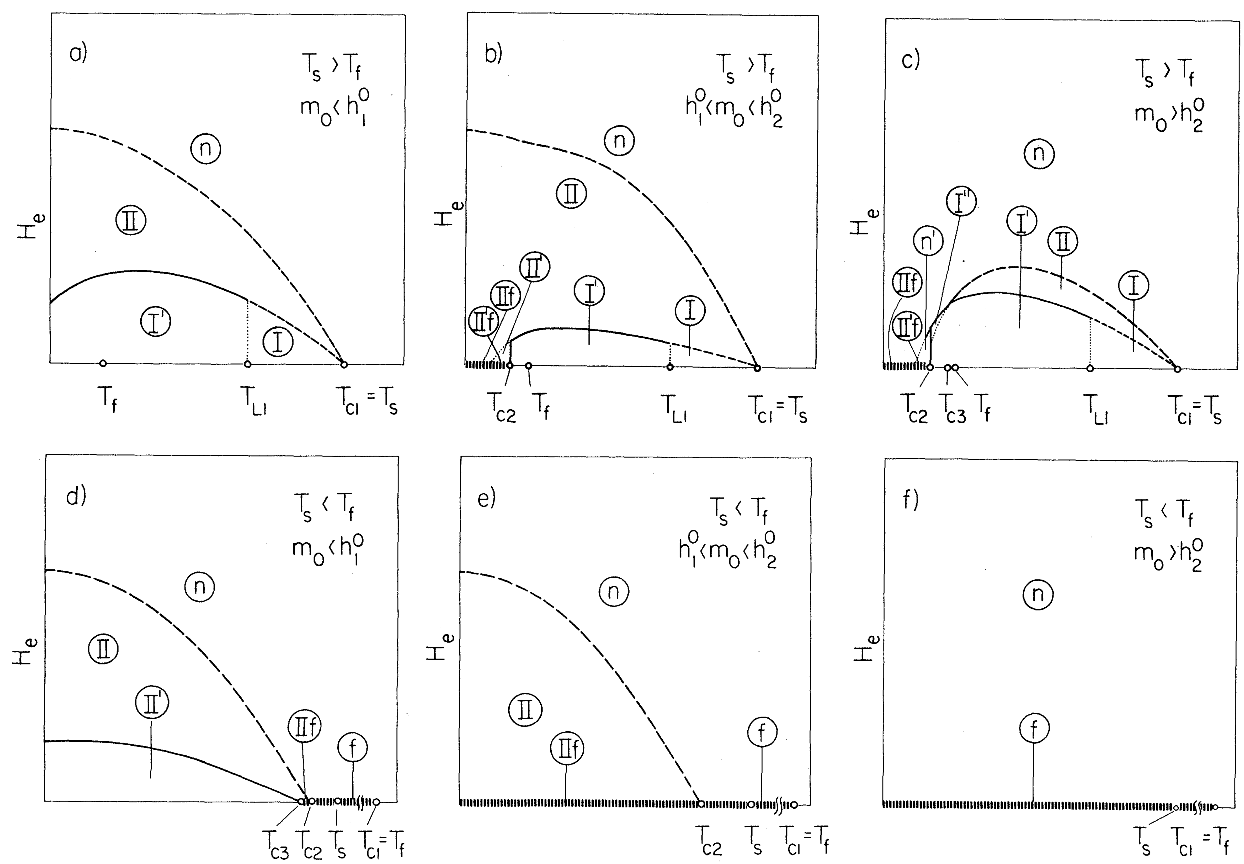

FIG. 1. Phase diagrams for the ferromagnetic superconductors, as described in the text. Temperature and external magnetic field axes are in arbitrary units.

is interesting to note that there are two temperatures, denoted T_{L1} and $T_{L2}=T_{c2}$, at which phase transitions change from being discontinuous to continuous.[13] The presence of the aforementioned regions of unstable phases may account, in part, for the hysteresis effects observed in the experiments.[1]

In order to further support a qualitative agreement between our theory and experiments[14] we note that this theory, even in such simple form, predicts a field-dependent zero-temperature magnetization. This occurs because $m_0 < h_2^0$ implying that even at $T = 0°K$ there is a negative contribution to the total magnetization originating from the superconductor. This contribution is annulled only at sufficiently high fields. The model predicts

$$M(H_{\mathrm{ext}}, 0) = m_0 + h_s(H_{\mathrm{ext}} + m_0, 0), \qquad (11)$$

which saturates to m_0 only for external fields satisfying

$$H_{\mathrm{ext}} \geq h_2^0 - m^0. \qquad (12)$$

Phase diagrams in Fig. 1 also imply that the behavior of FS's may range from superconductorlike (for $T_f \ll T_s$ and $m_0 \ll h_1^0$) to ferromagnetlike (for $T_f \gg T_s$ and $m_0 \gg h_2^0$) with a spectrum of intermediate cases. These cases include total destruction of superconductivity at the onset of long-range magnetic order [Fig. 1(c)] as well as complete destruction of ferromagnetism at the onset of superconductivity [Fig. 1(d)]. More peculiar cases may occur. For example, if $T_f \lesssim T_s$ and $m_0 \lesssim h_1^0$ then the theory predicts the possible occurrence of reentrant superconductivity in zero external field: The system would become superconducting below T_s in the small-temperature region of the order $(T_s - T_f)$, then it would become ferromagnetic only to become superconducting again at some yet lower temperature. Another intriguing question is whether superconductivity and ferromagnetism can coexist. We address it by analyzing the following condition:

$$M(0,T) \neq 0, \quad H_s(0,T) = -H_{\mathrm{ext},s}(0,T). \qquad (13)$$

This gives a temperature interval $T_1^* < T < T_2^*$ in which coexistence is possible. We found[9,11,12]

$$T_2^* = (1 - \lambda_f \lambda_s/\lambda) T_f, \qquad (14)$$

assuming $T_2^* < T_s$ (otherwise $T_2^* = T_s$). For the lower bound we find $T_1^* = 0°K$ if $h_1^0 > \lambda_f m_0$; otherwise it is given implicitly by the equation

$$h_1(T_1^*) = \lambda_f m_0 \tanh[T_2^* h_1(T_1^*)/\lambda_f m_0 T_1^*]. \qquad (15)$$

Therefore, our model leads to a natural conclusion that the coexistence is possible when coupling between magnetic moments is much stronger than coupling between the superconductor and the ferromagnet (i.e., $\lambda > \lambda_f \lambda_s$).

One of the serious shortcomings of a mean-field theory is that fluctuations are neglected.[15] Their importance will be considered in future work. The fluctuations of H_f, for example, should modify our results for the paramagnetic region, $T \approx T_s > T_f$, where scattering of superconducting electrons on disordered magnetic moments occurs. This scattering can be partially taken into account by a correction of T_s as given, for example, by the Gor'kov-Rusinov theory.[6]

In order to answer some of the above questions, a more detailed analysis of experimental data is in progesss.[9] Also, in the light of experiments on antiferromagnetic superconductors,[2] we are interested in extending this theory to accommodate them as well.

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[9]A longer paper including details of the calculations, as well as quantitative comparison with the experiments, is in preparation.

[10]We use definition of magnetization which includes a factor 4π.

[11]In a more general case screening fields in Eqs. (4) and (5) should be taken as $H_{ext}+\lambda_f H_f$ and $H_{ext}+\lambda_s H_s$, respectively. For simplicity we take $\lambda_f=\lambda_s=1$.

[12]The molecular field should be in general taken as λH_f.

[13]Because of the chosen infinite slope in h_s at $h=0$ [c.f. Eq. (7)], $T_{L1}=T_s$ in the present calculation.

[14]H. R. Ott, W. A. Fertig, D. C. Johnston, M. B. Maple, and B. T. Matthias, to be published.

[15]It is for that reason, for example, that in the calculation presented, the uppermost transition temperature is equal to the larger of T_s and T_f.

ERRATA

EXCITATION OF ATOMIC HYDROGEN TO THE $n=2$ STATE BY HELIUM IONS. Victor Franco [Phys. Rev. Lett. 42, 759 (1979)].

The left-hand side of Eq. (7) should read $F_{fi}(\vec{q}, k)$.

In the acknowledgement, "City University of New York Public Service Commission–Bureau of Higher Education research award" should be replaced by "grant from the PSC-BHE Research Award Program of the City University of New York."

FURTHER EVIDENCE FOR FRACTIONAL CHARGE OF $\frac{1}{3}e$ ON MATTER. George S. LaRue, William M. Fairbank, and James Douglas Phillips [Phys. Rev. Lett. 42, 142 (1979)].

There were several typographical errors in the set of residual charge values listed in the second column of page 144. These values as presented in Fig. 3, however, are correct. The list should have been as follows: Results reported in Ref. 1 are [1] $(-0.007\pm0.039)e$; [2] $(0.089\pm0.073)e$; [3] $(-0.331\pm0.070)e$; [4] $(-0.016\pm0.030)e$; [1] $(-0.015\pm0.054)e$; [3] $(0.060\pm0.092)e$; [5] $(-0.034\pm0.093)e$; [6] $(0.313\pm0.019)e$; [7] $(0.030\pm0.023)e$; [8] $(-0.001\pm0.026)e$; [6] $(0.327\pm0.010)e$. Results obtained since Ref. 1 are [6] $(0.016\pm0.024)e$; [6] $(0.304\pm0.040)e$; [6] $(-0.029\pm0.017)e$; [6] $(-0.026\pm0.016)e$; [7] $(0.023\pm0.015)e$; [9] $(0.325\pm0.043)e$; [7] $0e$ assumed; [9] $(0.361\pm0.040)e$.

On line 9, page 143, $\Delta E_{\rm Batt}$ should be replaced by $\Delta F_{\rm Batt}$ and on line 6 of the last paragraph on page 144 $-\frac{1}{3}e$ should be replaced by $+\frac{1}{3}e$.