Thus, $\nu/\alpha = -3, -1, 1, 3$ are end-point singularities[10] of A_0 and A_0' corresponding to end points of contour of integration $(k_x, k_y, k_z) = (0, 0, 0)$, $(0, 0, \pi)$, $(0, \pi, \pi)$, (π, π, π), respectively. To see the nature of these singularities we consider, for simplicity,

$$D_0 = \frac{1}{\pi^3} \iiint_0^{\pi} \frac{dk_x dk_y dk_z}{\nu/\alpha + \cos k_x + \cos k_y + \cos k_z} ,$$

which has the same analytic properties as the A's. Since

$$\frac{1}{\pi^2} \iint_0^{\pi} \frac{dk_x dk_y}{\nu/\alpha + \cos k_x + \cos k_y + \cos k_z}$$

$$\sim C_1(a) \ln(\nu/\alpha + \cos k_z - a) + C_2(a) \tag{B2}$$

for $\nu/\alpha + \cos k_z \sim a$, where $a = -2, 0, 2$, we observe that $D_0 \propto (\nu/\alpha - b)^{1/2}$ for $\nu/\alpha \sim b$, where $b = -3, -1, 1, 3$. Therefore the end-point singularities of A_0 and A_0' are all square-root branch points. It is well known that across the real axis between $\nu/\alpha = -3$ and 3, the imaginary parts of A_0 and A_0' change sign, while the real parts are continuous. So the branch cut lies on the real axis between -3 and 3, in the ν/α plane. Furthermore, there are two Riemann sheets for the part of the ν/α plane where $\mathrm{Re}(\nu/\alpha) < -1$.

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$$\cos(z \cos\phi) = J_0(z) + \sum_{n=1}^{\infty} (-1)^n J_{2n}(z) \cos 2n\phi$$

and obtain

$$\begin{aligned} M(k) &= \int_0^1 d(\cos\theta)\, J_0(k \sin\theta) \cos(k \cos\theta) \\ &= \int_0^1 x(1-x^2)^{-1/2} \cos[k(1-x^2)^{1/2}]\, J_0(kx)\, dx \\ &= (\sin \sqrt{2}k)/\sqrt{2}k \;; \end{aligned}$$

cf. E. T. Whittaker and G. N. Watson, *Modern Analysis* (Cambridge U. P., London, 1963).

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Cowley Theory of Long-Range Order in β-CuZn

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The Cowley theory is used to estimate the effect of nonstoichiometry on long-range order in β-CuZn alloys.

Accurate Ising-model calculations of the temperature dependence of long-range order in β-CuZn are available at the present only for the stoichiometric alloy.[1,2] To estimate the change in the long-range-order curve due to a departure from the stoichiometric composition, we have investigated the approximate theory of order developed[3] and revised[4] by Cowley. Although its thermodynamic formulation is not rigorous, we shall show that this theory does give a long-range-order curve for equiatomic β-CuZn in good agreement with Ising-model calculations except at the higher temperatures near T_c, and it can give the proper dependence on composition in the limit of low temperatures, so we suggest that it should give a reasonable estimate of the effect of nonstoichiometry over much of the range of temperature below T_c.

Cowley did not give an expression for long-range order in nonstoichiometric alloys in his papers. Our equations for the β-CuZn alloys are derived from his initial paper[3] after changing one approximation, which appears equivalent to using a simple form of the revised approach of his later papers.[4] Cowley developed an expression for the free energy in terms of the Warren short-range-order parameters α_l, which had been shown to have the limiting values

$$\alpha_L = \pm(1-\epsilon^2)S^2\,, \qquad (1)$$

where S is the long-range-order parameter as defined by Cowley, the atomic fraction of Cu atoms in the alloy has been written as $\frac{1}{2}(1+\epsilon)$, and the + sign is used for sites on the same sublattice as the origin and the − sign for sites on the other sublattice. Now, in minimizing the free energy for $S \neq 0$, we change his approximation that all the α_I are independent variables, assuming, instead, that S^2 is the independent variable and, ignoring local correlations, that $\alpha_I \simeq \alpha_L$ for all sites. The resulting equation, which combines terms from both sublattices, is easily manipulated to give

$$kT \ln\left\{\frac{1+(1-\epsilon)^2S^2}{1-(1-\epsilon)^2S^2}\left[\frac{1+(1-\epsilon^2)S^2}{1-(1-\epsilon^2)S^2}\right]^2\frac{1+(1+\epsilon)^2S^2}{1-(1+\epsilon)^2S^2}\right\}$$

$$= 4(1-\epsilon^2)S^2[8V_1 - 6V_2 + 12V_3 \cdots]\,, \qquad (2)$$

where V_i is the usual ith-neighbor interaction energy. Letting $S \to 0$ as $T \to T_c$, one finds

$$kT_c = \tfrac{1}{2}(1-\epsilon^2)[8V_1 - 6V_2 + 12V_3 \cdots]\,, \qquad (3)$$

and Eq. (2) can be written

$$\ln\left\{\frac{1+(1-\epsilon)^2S^2}{1-(1-\epsilon)^2S^2}\left[\frac{1+(1-\epsilon^2)S^2}{1-(1-\epsilon^2)S^2}\right]^2\frac{1+(1+\epsilon)^2S^2}{1-(1+\epsilon)^2S^2}\right\}$$

$$= 8S^2\,\frac{T_c}{T}\,. \qquad (4)$$

Equation (4) is the basic equation for long-range order in nonstoichiometric β-CuZn. It reduces properly to Cowley's equation for the equiatomic alloy,

$$\ln\left\{\frac{1+S^2}{1-S^2}\right\} = 2S^2\,\frac{T_c}{T} \qquad (5)$$

when $\epsilon = 0$. It is symmetric in ϵ, and as $T \to 0$ it predicts the limiting value

$$S_0 = 1/(1+|\epsilon|)\,, \qquad (6)$$

which is the maximum value that the parameter S can have in an alloy of that composition. As $T \to T_c$ it gives the asymptotic relation

$$S = \frac{3^{1/4}}{(1+3\epsilon^2)^{1/2}}\left(\frac{T_c}{T} - 1\right)^{1/4}\,, \qquad (7)$$

which is only weakly dependent on ϵ.

TABLE I. Comparison of the long-range-order parameters $S(\epsilon)$ for equiatomic β-CuZn ($\epsilon = 0.00$) and for the alloy with 52 at.% Cu ($\epsilon = 0.04$).

T/T_c	$S(0.00)$	$S(0.04)$	$S(0.04)/S(0.00)$
0.4	0.9928	0.9615	0.9685
0.5	0.9785	0.9589	0.9800
0.6	0.9525	0.9425	0.9894
0.7	0.9103	0.9046	0.9937
0.8	0.8429	0.8393	0.9958
0.9	0.7249	0.7226	0.9969
1.0	0.0000	0.0000	0.9976

Let us first compare the long-range-order curve for the equiatomic alloy with the recent Ising-model calculations of Essam and Fisher[1] and of Baker and Essam.[2] There clearly will be significant differences for temperatures near T_c, since the Cowley theory shows S varying as the reduced temperature raised to the power 0.25, while the two Ising calculations give exponents of 0.30 and 0.31. However, at lower temperatures the agreement is surprisingly good; the value of S from Eq. (5) agrees with that from the [10, 10] Padé approximant of Essam and Fisher to better than 1% for $T/T_c \leq 0.84$, and it agrees with the "compressible" model calculation of Baker and Essam to within 2.3% for all $T/T_c \leq 0.95$.

Now let us compare the long-range-order curve for an alloy containing 52 at.% Cu ($\epsilon = 0.04$) with that for the equiatomic alloy to illustrate the predictions of Eq. (4). The values of the long-range-order parameter $S(\epsilon)$ for these alloys and their ratio are given in Table I as a function of T/T_c. At low temperatures the long-range-order parameter for the nonstoichiometric alloy is appreciably smaller, but it is here also much less temperature dependent, so the effect of the nonstoichiometry decreases rapidly with increasing temperature and is an order of magnitude less near T_c. The effect of nonstoichiometry on the usual normalized order parameter S/S_0 is then of the opposite sense; nonstoichiometry *increases* this parameter by an amount varying from zero at $T = 0$ °K to a maximum at T_c.

Finally, it is interesting to compare these predicted effects with the discrepancies observed between our recent experimental measurements[5,6] (on an alloy with 51.9 at.% Cu) and the Ising-model calculations. The effect is of the appropriate sign to bring the theory and experiment closer together, but, as Domb[7] has suggested, it is too small to account for the observed differences, which are approximately three times the predicted effects on S/S_0 near T_c.

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Hyperfine Fields in Dilute Alloys of Co in Fe

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Spin-echo NMR spectra of ^{57}Fe and ^{59}Co in Fe alloys with 0.8, 2.6, 3.3, and 6 at.% Co have been decomposed to determine the influence of Co atoms on nearby Fe and Co hyperfine fields as a function of radial separation. Of the possible alternatives, the preferable solution of this long-standing question is similar, for the Fe sites, to that of Wertheim, Buchanan, and Wernick, but with second-nearest-neighbor effects only one-half as great. The model is interpreted in terms of an oscillatory radial variation affecting all sites, combined at Fe sites with changes in local moments to yield an over-all monotonic variation in hyperfine field with distance from Co atoms.

The distribution of Fe hyperfine fields in dilute alloys of cobalt in iron has been the subject of numerous NMR and Mössbauer-effect studies. While the experimental results are in substantial agreement, the interpretations have not been, despite reliance on a common model.[1] This paper is a further attempt to rectify this situation using NMR data for higher Co concentrations than reported elsewhere,[1,2] and with greater resolution than is available in Mössbauer studies.[3] The effects of Co impurities on Fe hyperfine fields are found to be about the same as those given by the more recent interpretations, although second-nearest-neighbor effects come out significantly smaller. A connection is also made with the Co hyperfine fields in the same alloy system.

In the generally used model, the effects of Co impurities are taken to depend only on distance (i.e., all Co impurities on a given spherical shell of neighboring sites are equivalent), and the effects of impurities are additive. With the further assumption that the Co atoms are distributed at random, one identifies observable features of the spectra using intensities calculated from the probabilities of occurrence of various near-neighbor configurations. Only a few neighbor shells, on the order of four, appear to be important in accounting for the main features of the hyperfine field spectra of dilute Fe alloys, in agreement with the range of perturbations established by neutron diffraction.[4]

Early pulsed-NMR studies[5] attributed the single distinct Fe satellite line found with low Co concentrations to an impurity in the nearest-neighbor shell and assumed that farther shells caused small perturbations. Analyses of unresolved Mössbauer spectra found larger shifts,[6] and Wertheim[3] pointed out that the change of Mössbauer peak position with concentration also implies that there must be hyperfine field shifts of greater magnitude. The cw NMR work of Mendis and Anderson[2] with very low Co concentrations suggests that the observed satellite is the result of a more distant neighbor, identified as the third neighbor. The first- and second-shell effects were presumed to be greater, but broadened beyond observability, a limitation not shared by the Mössbauer work. Recent spin-echo traces of a 1% sample by Budnick *et al.*[1] show evidence of these greater shifts, while Mössbauer work by Wertheim *et al.*,[3] analyzed for the effects of four shells of neighbors, agrees with the assignments by Mendis and Anderson. In all of these interpretations auxiliary conditions are imposed to obtain unique solutions. It has generally been assumed that the effects decrease monotonically with distance; this is particularly important for Mössbauer studies where no features are resolved.

This paper reports an examination of zero-field, 4.2 °K, spin-echo NMR spectra of Fe:Co alloys without the above constraint. Both ^{57}Fe and ^{59}Co spectra of samples containing 0.8, 2.6, and 3.3 at.% Co were studied. The Co resonance of a 6 at.% sample was also used; the corresponding Fe signal was unusable. These traces were the basis for an earlier report,[5] but have been reexamined in light of later developments.

The experimental results for ^{57}Fe are shown as points in Fig. 1, as are the corresponding spectra for ^{59}Co in Fig. 2. Corrections for relaxation-time variations were unnecessary and frequency-dependent amplitude variations are small enough