Interaction between the d-Shells in the Transition Metals. III. Calculation of the Weiss Factors in Fe, Co, and Ni*

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Estimates are made of the Weiss factors for Fe, Co, and Ni using the author's previously proposed theory of indirect coupling via the conduction electrons. In this estimate use is made of only (i) the spectroscopic data for the coupling between the spin of the outer $4s$ electron and the spin of the inner incomplete $3d$ shell for the isolated atoms, (ii) the Hartree solution for the isolated Fe atom, (iii) the assumption that the conduction electrons behave as a free electron gas, (iv) the assumption that the direct coupling between adjacent d shells is negligible. The computed Weiss factors increase in the series Fe, Co, Ni in the same manner as do the empirical factors, but are somewhat larger. This discrepancy is in the right direction demanded by the previously proposed postulate that the direct interaction between adjacent d-shells always tends to an antiferromagnetic alignment.

I. INTRODUCTION

IN the first paper[1] of this series the author proposed that ferromagnetism in metals arises from an indirect coupling between incomplete d-shells via the conduction electrons, rather than from the usually assumed direct coupling. The evidence given in favor of this proposal was primarily of a qualitative nature. In the present paper this proposal is subjected to the quantitative test of the estimation of the Weiss factors for Fe, Co, and Ni using only this indirect coupling via the conduction electrons. The estimates, summarized in the seventh row of Table II, are found to be consistent with the empirical values of the Weiss constants (eighth row). The estimated values are, however, somewhat larger than the empirical values, in accord with the previously proposed viewpoint that the neglected direct interaction between d-shells always leads to a negative contribution to the Weiss factors.

II. ANALYSIS AND RESULTS

The basis of the Weiss phenomenological theory of magnetism is the assumption that the interaction between the elementary magnetic moments may be described by an effective magnetic field, H_{eff}, which contains, besides the applied field, H, a term proportional to the magnetization intensity J. Thus, one obtains

$$H_{eff} = H + WJ. \tag{1}$$

The constant of proportionality W is now known as the Weiss factor. Its values for the ferromagnetic metals Fe, Co, and Ni are given in Table I. One of the objectives of any theory of ferromagnetism must be the evaluation of these Weiss factors.

In order that we may readily compare W with theoretical quantities, we desire W in an energy equation rather than in Eq. (1) for H_{eff}. Towards this end we observe that, according to this equation, the energy of interaction between the elementary magnetic moments is given by

$$E_{spin} = -(1/2)WJ^2 \text{ per cm}^3. \tag{2}$$

If we now define S_d as the mean component, along the direction of magnetization, of the spin of each incomplete d-shell expressed in units of a Bohr magneton μ_B, we obtain

$$E_{spin} = -(1/2)W'S_d^2 \text{ per atom}. \tag{3}$$

The new Weiss factor W' is related to the original W by

$$W' = N\mu_B^2 W, \tag{4}$$

where N is the number of atoms per unit volume. This new Weiss factor is likewise given in Table I.

On comparing Eq. (3) above with Eq. (3) of reference 1, we obtain the following relation:

$$W' = (\beta^2/\gamma) - \alpha \tag{5}$$

between W' and the fundamental constants of our theory of ferromagnetism. These constants are defined as the coefficients in the equation

$$E_{spin} = (1/2)\alpha S_d^2 - \beta S_d S_c + (1/2)\gamma S_c^2, \tag{6}$$

where S_c is the mean magnetization, in units of Bohr magnetons per atom, of the conduction electrons.

The coefficient α is proportional to the direct exchange interaction between adjacent d-shells. In our current theory of ferromagnetism we do not assume, as is customary, that this coefficient changes sign as the overlap between adjacent d-shells diminishes, but merely assume that α decreases continuously. Thus, as we pass to the right along the first transition period, α becomes smaller than the first term in Eq. (5). In the absence of a direct evaluation of α we shall neglect

TABLE I. Weiss factors.

	Fe	Co	Ni
W (in ergs)	6160[a]	7700[a]	13,400[a]
W' (in ev)	0.028	0.036	0.065

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[1] C. Zener, Phys. Rev. **81**, 440 (1951).

[a] R. Becker and W. Döring, *Ferromagnetismus* (Verlag. Julius Springer, Berlin, 1939), p. 27.

Table II. Ferromagnetic coupling coefficients (in units of ev).

	Fe	Co	Ni
Configuration	$3d^7(^4F)4s$	$3d^8(^4F)4s$	$3d^9(^2F)4s$
β_0	0.104	0.125	0.148
β	0.34	0.41	0.48
γ_{KE}	7.8	5.5	5.9
γ_{ex}	−5.5	−2.7	−3.0
γ	2.3	2.8	2.9
β^2/γ	0.050	0.060	0.081
W'	0.028	0.036	0.065

it entirely. We thereby obtain an upper limit to the theoretical value of W'.

An estimate of β may be obtained from spectroscopic data of the isolated atoms, and from a knowledge of how the outer $4s$ electron is constrained to spend more time in the vicinity of the $3d$ shell as the atoms condense from the vapor to the solid phase. The configuration of the isolated Fe atom is $3d^6\,4s^2$. On demotion of one of the $4s$ electrons the state becomes $3d^7(^4F)4s$. Corresponding to the remaining $4s$ electron having a spin parallel or antiparallel to that of the core, we have a ^5F or a ^3F state. The former state lies lower than the latter by 0.624 ev.[2] If we now represent the spins, in units of μ_B, of the $3d$ and $4s$ shell by S_d and S_s, and their coupling energy by

$$-\beta_0 S_d S_s,$$

we thereby obtain that β_0 is equal to 0.104 ev. In a corresponding manner we find that the coupling coefficients β_0 appropriate to Co and Ni isolated atoms are 0.125 and 0.148 ev, respectively. In the isolated atom the $4s$ electron spends the major part of its time outside of the $3d$ shell. When the atoms condense to the solid
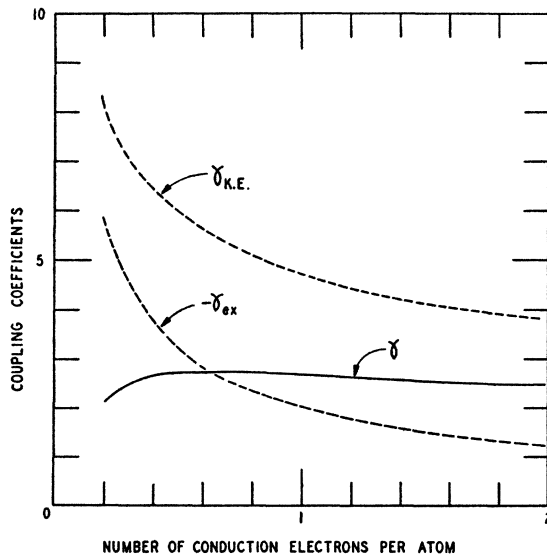

FIG. 1. Illustration of the insensitivity of γ to the number of conduction electrons per atom. Computed for example of Fe.

NUMBER OF CONDUCTION ELECTRONS PER ATOM

phase, the $4s$ electrons become conduction electrons, and spend a greater fraction of their time within the region of the d shells. The coupling coefficient β between the spins of the conduction and the $3d$ electrons is correspondingly increased over the coupling coefficient β_0 characteristic of the isolated atoms. In order that we may estimate the ratio β/β_0, we inquire as to what fraction, f, of the time a $4s$ electron in an isolated atom spends within a spherical surface of such a radius r_s as to enclose a volume equal to the atomic volume of the condensed phase. We shall then set

$$\beta = \beta_0/f.$$

This fraction f may be obtained directly from the Hartree self-consistent calculations for the function $Z_{4s}(r)$. Thus, in the case of Fe, with two $4s$ electrons,

$$f = (1/2)\{2 - Z_{4s}(r_s)\}.$$

On using the value $2.66a_0$ for r_s, we find from the tables for Fe given by Manning and Goldberg[3] that $Z_{4s}(r_s)$ is 1.39, and hence f is 0.305. For Fe we shall therefore take

$$\beta/\beta_0 = 3.28.$$

In the absence of Hartree solutions for Co and for Ni, we shall take a similar ratio for these metals. The values of β so computed are given in Table II.

Two distinct factors contribute to the coefficient γ. The first factor arises from that increase in the Fermi kinetic energy which is associated with a polarization of the conduction electrons. This first factor gives the positive contribution

$$\gamma_{KE} = (10/9)\bar{\varepsilon}_K/v,$$

where $\bar{\varepsilon}_K$ is the average Fermi kinetic energy, and v is the number of conduction electrons per atom. The second factor arises from that change in the correlation energy of the conduction electrons which is associated with their polarization. The dominant part of this correlation energy is the exchange energy[4] between electrons of like spin. This exchange energy gives the negative contribution

$$\gamma_{ex} = (4/9)\bar{\varepsilon}_{ex}/v,$$

where $\bar{\varepsilon}_{ex}$ is the exchange energy per conduction electron. In computing γ we shall adopt the model of a free electron gas for the conduction electrons, and therefore take[5]

$$\bar{\varepsilon}_{KE} = 21.82n^{\frac{2}{3}}\ \text{ev}, \quad \bar{\varepsilon}_{ex} = 10.81n^{\frac{1}{3}}\ \text{ev},$$

where n is the number of conduction electrons per A^3. Whereas both γ_{KE} and γ_{ex} are sensitive to the assumed value of v, their sum γ is quite insensitive, as is illus-

[2] R. F. Bacher and S. Goudsmit, Atomic Energy States (McGraw-Hill Book Company, Inc., New York, 1932).

[3] M. Manning and L. Goldberg, Phys. Rev. 53, 662 (1938).
[4] F. Seitz, Modern Theory of Solids (McGraw-Hill Book Company, Inc., 1940), p. 341.
[5] P. Gombas, Die Statistische Theorie des Atoms (Verlag. Julius Springer, Wien, 1949), pp. 7 and 25.

trated in Fig. 1. In the calculation given in Table II, v was taken as 0.22, 0.7, 0.6 for Fe, Co, and Ni, respectively, these values being required by the observed values of the saturation magnetization.

The calculated ratio β^2/γ is compared with the empirical W' in the last two rows of Table II. In spite of the approximate nature of the estimates leading to the values for β^2/γ, these values are satisfying in two respects. As we pass from Fe through Co to Ni, β^2/γ increases in approximately the same manner as does W'. For each metal the calculated β^2/γ is somewhat larger than the empirical W', thereby allowing for a negative contribution from the coefficient α. We conclude that the model for ferromagnetism proposed in the first paper of this series gives a satisfactory quantitative interpretation of the Weiss constant.

A Variational Approach to Nuclear Reactions

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The formalism of Wigner and Eisenbud for nuclear reactions is carried out by means of a variation principle. A variation principle of the Hulthén type is derived for the R matrix and applied to trial wave functions written in terms of the resonance functions, X_λ, of the Wigner-Eisenbud formalism. As a result, a finite level formula for the R matrix is directly obtained.

I. INTRODUCTION AND SUMMARY

IN a paper by Wigner and Eisenbud,[1] general equations describing nuclear reactions are rigorously derived. The essential result of the theory is the expression which the authors obtain for a matrix which they call the R matrix. The R matrix is a real, symmetric matrix whose rows and columns are labeled according to the possible alternatives of the reaction. From the R matrix one may directly calculate the collision matrix, which gives the cross sections of the possible reactions according to $\sigma_{ss'} = \pi k_s^{-2} |\delta_{ss'} - U_{ss'}|^2$, where $\sigma_{ss'}$ is the cross section of the reaction going from the sth pair of particles to the s'th pair and $U_{ss'}$ is the corresponding element of the collision matrix. The R matrix is related to the collision matrix of the reaction by an equation of the form $U = \omega(1 + ijRj)(1 - ijRj)^{-1}\omega$, where j and ω are, respectively, real diagonal and unitary diagonal matrices. The elements of the j and ω-matrices depend only on non-nuclear parameters, in that they involve only constants which enter into the solutions of the two-body Schrödinger equation in the regions of configuration space where there are two distinct reaction products. The calculation of the collision matrix from the R matrix may therefore be accomplished in a straightforward manner without any additional information about the compound nucleus other than that which is contained in the R matrix. This paper will concern itself only with the R matrix.

An expression for the R matrix will be obtained on the basis of a variational calculation. The variation principle is of the same general type as that derived by Hulthén[2] for the two-body quantum-mechanical scattering problem. The derivation presented here is along lines similar to those followed by W. Kohn[3] in a recent paper.

The variation principle is applied to a trial wave function, which is written in terms of a finite number of functions, X_λ, defined in W-E. These functions are intended to represent the resonance states of the compound nucleus. Upon making the variational expression stationary with respect to variations of the coefficients of the X_λ, one obtains directly an expression for the R matrix in terms of the states used in the trial wave function. The variationally derived expression for the R matrix is in agreement with the rigorous expression for the R matrix up to the order of the number of terms used in the trial wave function. Moreover, the variationally derived R matrix is real and symmetric for all trial wave functions of the type considered.

The notation used in this paper will be essentially the same as the notation of W-E. This has two advantages. First, it gives the present work all of the generality of W-E in that arbitrary long-range interactions and arbitrary angular momenta are allowed. Second, it allows for a direct comparison between the results of the variational calculation and the rigorous result.

In order to carry out this work it will be necessary to present a brief description of the Wigner-Eisenbud formalism. This will be done in Sec. II. Section III is

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[1] E. P. Wigner and L. Eisenbud, Phys. Rev. **72**, 29 (1947). This reference will be referred to as W-E throughout the remainder of this work.

[2] L. Hulthén, Extrait, Dixième Congrès des Mathematiciens Scandinaves, Copenhague, 1946.

[3] W. Kohn, Phys. Rev. **74**, 1763 (1949).