Magnetic Interaction in Heusler Alloy

The ferromagnetic alloy of manganese, copper and aluminum, discovered by Heusler,[1] is now regarded[2] as a superstructure alloy having the ideal composition Mn Cu_2 Al, the manganese atoms being in face-centered cubic arrangement with $a=5.950\times10^{-8}$ cm. If the permanent magnetic moment present is, as usual, wholly ascribed to manganese atoms the magnetic moment per atom may be taken as $P=3.14\times10^{-20}$ (gaussian units), corresponding to a saturation magnetization $I_{\max}+580$. Even higher values than this have been advocated.[3]

These data permit a calculation of magnetic interaction and resultant ferromagnetic anisotropy, as explained in a recent paper.[4] The following numerical values of quantities listed in Table III of that paper are obtained: $P\times10^{20}=3.14$; $2\rho a=1.71\times10^{-8}$ (Slater[5]); $N=4$; $a\times10^{8}=5.950$; $\rho=0.144$; $\lambda=0$; $F_4=-0.1244$; $F_6=0.0145$; K_1 (quadrupole part) $=+0.42$; K_1 (sextupole part) $=-0.36$; K_1 (total) $=+0.06$; K_2 (sextupole) $=+3.96$ (all K_n in 10^6 erg·cm^{-3}).

The experimental work available for comparison[6] has been interpreted[7] as giving $W_{110}-W_{100}=-0.224\times10^6$ erg·cm^{-3}, corresponding to $K_1=-0.9\times10^{-6}$ erg·cm^{-3}. Nothing is known about K_2.

The theory at this stage agrees with experiment only in giving a small absolute magnitude for K_1. The disagreement of signs could be removed by supposing an expansion of the 3*d* electron shell of manganese in the alloy (increase in ρ), which would allow the sextupole contribution, proportional to ρ^4, to increase with respect to the quadrupole contribution, proportional to ρ^2. The high value of P negatives the hypothesis $\lambda=0$ which would otherwise be attractive, since it gives $F_4=+0.2488$; $F_6=+0.0516$; K_1 (quadrupole part) $=-0.84$; K_2 (sextupole part) $=-1.28$; K_1 (total) $=-2.12$.

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[1] F. Heusler, Verh. d. D. phys. Ges. **5**, 220–223 (1903).
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[3] S. Valentiner and G. Becker, Zeits. f. Physik **83**, 371–403 (1935), suggest 20 Weiss magnetons per atom, that is, $P=3.71\times10^{-20}$ (gaussian units).
[4] L. W. McKeehan, Phys. Rev. **52**, 18–30, 527 (1937).
[5] J. C. Slater, Phys. Rev. **36**, 57–64 (1930), column (5), Table I (d), p. 62.
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On the Lower Bounds of Weinstein and Romberg in Quantum Mechanics

Weinstein[1] has proposed as a lower bound for the lowest eigenvalue the expression $I_1-(I_2-I_1^2)^{\frac{1}{2}}$, where

$$I_1=\int\psi H\psi d\tau,\qquad I_2=\int(H\psi)^2d\tau,$$

ψ being any (normalized) approximate wave function, and the usual notation being used. This result has not been accepted as being rigorously proved, however, and Romberg[2] has given an example purporting to show that Weinstein's expression may lead to wrong results. Romberg has also proposed the expression $-(I_2)^{\frac{1}{2}}$ as a lower bound. It can, however, be shown that Weinstein's lower bound (or rather a generalization of it) holds rigorously when the conditions for its validity are properly formulated. Romberg's example of apparent failure is, in fact, fallacious. We wish to point out also that a more advantageous use can be made of the constant denoted below by α.

Let the function ψ satisfy the following conditions: (a) ψ satisfies the boundary conditions of the problem,[3] (b) both ψ and $H\psi$ are expansible in series of eigenfunctions which converge "in the mean".[4] Further, let α be a real constant satisfying $E_0<\alpha\leqq(E_0+E_1)/2$, where E_0 is the lowest eigenvalue and E_1 that immediately above. Then it follows rigorously from the "completeness relation" [4] for $(H-\alpha)\psi$ that

$$E_0\geqq L,\qquad L=\alpha-(I_2-2\alpha I_1+\alpha^2)^{\frac{1}{2}}. \qquad (1)$$

In order that condition (b) may hold, it is necessary that the integrals I_1, I_2 should exist, and it is practically certain that the existence of these integrals, together with condition (a), is also *sufficient* for (b) to hold.[5] Accepting this, (1) holds for any function such as is commonly used in the Ritz method. If, but only if, $H\psi$ also satisfies the boundary conditions, we may write $I_2=\int\psi H^2\psi d\tau$. This is often *not* the case.

Excluding the trivial case that ψ is an *exact* eigenfunction, L, as a function of α, increases steadily from $-\infty$ to I_1 as α increases from $-\infty$ to $+\infty$. Hence we can remove the condition $\alpha>E_0$ and require merely $\alpha\leqq(E_0+E_1)/2$. Weinstein takes $\alpha=I_1$, which is permissible if ψ is at all a good approximation to the correct eigenfunction; but the *best* choice is obviously that which makes L a maximum, namely $\alpha=(E_0+E_1)/2$. Romberg's expression is obtained with $\alpha=0$, which is certainly *not* a permissible value if—as in most problems—E_0 and E_1 are both negative. In the opinion of the writer, no reliance can be placed on Romberg's expression, for (unlike (1)) it depends on the zero of energy. Further, it definitely fails in some cases.

The logical procedure is first to make a definite choice of α, selecting the greatest value for which the inequality $\alpha\leqq(E_0+E_1)/2$ is safely satisfied, and then to determine ψ so as to make L a maximum, i.e.,

$$I_2-2\alpha I_1=\text{minimum}.$$

Other choices of α give an upper bound for E_0, or upper and lower bounds for the higher eigenvalues, as given by Weinstein. The upper bound for E_0, however, offers no advantage over the Ritz approximation. It is intended to discuss some of the above points in greater detail in a future paper, and also to apply the method to derive a rigorous lower bound for the normal state of helium.

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[1] D. H. Weinstein, Proc. Nat. Acad. Sci. **20**, 529 (1934), and previous papers cited there. See also J. K. L. MacDonald, Phys. Rev. **46**, 828 (1934).
[2] W. Romberg, Physik. Zeits. Sowjetunion **8**, 516 (1935).
[3] For a precise statement of these, see Pauli, *Handbuch der Physik*, second edition, Vol. 24/1, p. 121 *et seq.*, or the original paper of von Neumann cited there.
[4] For an explanation of this term, see, e.g., Courant and Hilbert, Methoden d. math. Phys., p. 42 *et seq.*, or Pauli, reference 3, p. 127 *et seq.*, where the extension to continuous spectra is also considered.
[5] This is really implicitly assumed in, for instance, using perturbation theory when the perturbation has singularities. A proof can be given in the case of a *finite* region by a modification of the argument used in Courant-Hilbert, reference 4, p. 368 *et seq.*, but the extension necessary to cover the case of an infinite region and continuous spectra, though plausible, presents difficulties, and has not yet (so far as the writer is aware) been given.