[4]S. R. Broadbent and J. M. Hammersley, Proc. Cambridge Phil. Soc. 53, 629 (1957).

[5]Review articles are H. L. Frisch and J. M. Hammersley, J. Soc. Indust. Appl. Math. 11, 894 (1963); M. E. Fisher, *Proceedings of the IBM Scientific Computing Symposium on Combinatorial Problems*, 1964 (IBM Data Processing Division, White Plains, N. Y., 1966), p. 179.

[6]M. E. Fisher and J. W. Essam, J. Math. Phys. 2, 609 (1961).

[7]P. W. Kasteleyn and C. M. Fortuin, J. Phys. Soc. Japan Suppl. 26, 11 (1969).

[8]R. B. Griffiths, J. Math. Phys. 8, 484 (1967).

[9]H. L. Frisch, S. B. Gordon, V. A. Vyssotsky, and J. M. Hammersley, Bell System Tech. J. 41, 909 (1962).

[10]M. E. Fisher in Ref. 5.

[11]M. F. Sykes and J. W. Essam, Phys. Rev. Letters 10, 3 (1963); J. Math Phys. 5, 1117 (1964).

[12]M. F. Sykes and J. W. Essam, Phys. Rev. 133, A310 (1964).

[13]M. E. Fisher, at the Statistical Mechanics Meeting of the Belfer Graduate School of Science, December, 1969 (unpublished).

[14]The computer work was carried out using the Univac 1108 computer at the Computer Center of the State University of New York at Albany.

[15]Which fact may be taken as an indication that fluctuations in the data due to the proximity of the critical point are insignificant.

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Effects of Hydrostatic Pressure on the Magnetic Ordering of Heavy Rare Earths*

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The effects of hydrostatic pressure on the magnetic ordering of heavy rare earths are studied through the pressure shift of the electronic energy bands and the effects of this pressure shift on the indirect exchange. It is shown that the change in the ordering temperature of Gd, Tb, and Dy and the variation of the helical turn angle of Tb can be explained in this manner.

Many experiments have been performed to study the effects of hydrostatic pressure on the magnetic ordering of heavy rare earths.[1-6] Below a certain critical pressure where a crystallographic transition takes place, the magnetic ordering temperature of Gd, Tb, Dy, and Ho was found to decrease linearly with pressure by the order -1 K/kbar. The type of initial magnetic ordering is unchanged by pressure, i.e., just below the ordering temperature Gd is ferromagnetic while Tb, Dy, and Ho are antiferromagnetic.[4,6] However, neutron diffraction experiments have revealed a reduction of helical turn angle in Tb and Ho when pressure is applied.[6] The purpose of our work is to explain these results from the point of view that the magnetic ordering of these metals is to a large extent determined by their electronic energy bands and Fermi-surface geometry.[7-9] It will be shown that this approach does give a quantitative understanding of the observed effects.

The program of our study proceeds by first calculating the electronic energy bands of the metal under study, then computing the generalized susceptibility function $\chi(\vec{q})$ for a $\vec{q}$ vector along the c axis, and finally correlating the location and the size of the peak of $\chi(\vec{q})$ with the magnetic ordering properties. This is done for Gd, Tb, and Dy under 0 and 20 kbar of pressure. The pressure effects are deduced from the shift of the $\chi(\vec{q})$ curve. In the following paragraph we explain briefly these calculations.

We used the relativistic augmented-plane-wave (RAPW) method for the energy band calculation,[10] the details of which are given in Ref. 7. The crystal potential was approximated by a muffin-tin potential constructed from a superposition of atomic potentials including the full Slater exchange. The lattice parameters under pressure were deduced from the elastic constants of Gd,[11] Tb,[12] and Dy.[13,14] Their actual values are listed in Table I. The radius of the augmented-plane-wave (APW) sphere was chosen as 3.32 a.u. for Gd and as 3.16 a.u. for Tb and Dy. The same APW sphere radius was used for both the zero-pressure and the 20-kbar calculations. We selected a set of 32 plane waves as the basis functions so that the band calculation was convergent to within 0.002 Ry. Energy eigenvalues were calculated over a mesh of 147 points in 1/24th zone. The spline interpolation method was used to interpolate the bands over a mesh of 450 000 points in the full zone. The susceptibility calculation was fully described in Ref. 9. With the interpolated bands, we calculated $\chi(\vec{q})$ for $\vec{q}$ along $\Gamma A \Gamma$ in the double zone scheme over a