H_{rf} and H_{dc}) as expected for a spin-wave resonance.

At $T = 110$ K a second absorption begins to occur at higher fields (see Fig. 2). The second absorption is very broad and occurs also at lower temperatures when H_{dc} is rotated several degrees from the a axis. Present theory offers no satisfactory explanation for the absorption peaks observed for H_{dc} aligned from 3° to 10° from the a axis in the basal plane of the sample when $T < 140$ K, which will be discussed in a later publication.

A second discrepancy between theory and experiment is that no absorption peak is observed when H_{dc} is aligned exactly along the a axis, contrary to the prediction of Cooper's free-lattice model.[1] Our experimental results reveal that peaks with the temperature dependence predicted by Cooper for the free-lattice model actually occur for H_{dc} from 1° to 2° off the a axis (see Fig. 1).

In conclusion, our results at 24 GHz experimentally confirm free-lattice-model behavior in Tb at low microwave frequencies where the $q = 0$ mode can be excited as predicted by Vigren and Liu, furnishing a satisfying resolution to the previously paradoxical ferromagnetic resonance data on terbium.

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Quadrupole Coupling Constants of Fe^{3+} in Yttrium Iron Garnet*

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The recently determined value of the quadrupole moment of Fe^{57m} has been shown to explain consistently the observed quadrupole coupling constants associated with two nonequivalent Fe sites in yttrium iron garnet.

In a previous publication[1] the molecular-orbital method for a complex imbedded in a lattice has been shown to resolve the ferrous-ferric anomaly in the quadrupole moment of Fe^{57m} by considering the cases of Fe_2O_3 and Al_2O_3:Fe^{3+}. It has also been established that the quadrupole moment of the iron nucleus is 0.18 b within 10% accuracy. However, it is still not clear whether this value of the quadrupole moment can also explain the observed quadrupole coupling constants in a variety of systems without fitting[2,3] with parameters such as polarizability and antishielding factors. The aim of this work is to examine this and present the results for yttrium iron garnet. This choice is made because (i) it is a complex structure with 160 atoms in a unit cell[4] (if our calculations can explain the quadrupole-coupling data in this case, we shall have hope of explaining the data in other cases); (ii) its crystal structure parameters are known very precisely[5]; (iii) there are two nonequivalent Fe sites {tetrahedral [24(*d*)] and octahedral [16(*a*)]} for which the Mössbauer spectra[6,7] have been observed; and (iv) the quadrupole coupling constants for both sites are known at room temperature.[6] This is essential since the precise crystal structure parameters available are determined at room temperature.

The calculation of the electric field gradient at the two iron sites has been performed in a manner outlined previously.[1,8] For the crystal structure parameters we use the refined values given by Euler and Bruce.[5] The wave functions[9,10] for Fe^{3+} and O^{2-} for the calculation of overlap and two-center integrals[11] are kept the same as in Ref. 1. Retaining the notations of Refs. 1 and 8 we present the various calculated field-gradient components in Table I for both tetrahedral [24(*d*)] and octahedral [16(*a*)] Fe sites (primes designate the components without antishielding effects). The total "local" contribution to the field gradient arising from the distortion of 3*d* etc. orbitals of Fe^{3+} due to overlap effects of 2*p* and 2*s* orbitals of the ligand O^{2-} is denoted by q_l'. Similarly, the symbols q_{nl}' and q_d' stand for the total "nonlocal" and "distant" contributions to the electric field gradient; q_{dB}', q_n', and q_{RL}' are the distant contributions from the bonding orbitals, the charges on the ligand nuclei, and the charges on the rest of the lattice, respectively. In q_{RL}' only the monopole contributions have been considered since the dipole contributions are negligible as is seen[1,8] in Al_2O_3, Fe_2O_3, and Al_2O_3:Fe^{3+} where these are 1.3, 0.016, and 0.40% of the corresponding total electric field gradients, respectively. The convergent sums for q_{RL}' have been obtained by forming neutral groups[12] in the crystal and summing the results from the groups lying within a sphere of radius R equal to $15a$, where a is the cell dimension. The sums are found to be convergent (with error less than 4 parts in 10^4) after taking the contributions from within a sphere of $R=3a$ for an octahedral site and $R=11a$ for a tetrahedral site. The reason for the difference in convergence is partly due to the fact that in the case of an octahedral Fe site the electric field gradient from yttrium ions [24(*c*)] exactly cancels that from the iron ions at tetrahedral locations [24(*d*)]; also, the contributions from the iron ions at octahedral locations [16(*a*)] sum up to zero. The arrangement of oxygen ions [96(*h*)] relative to the two sites is also responsible for this behavior. It is worth pointing out that the field gradients (including nearest-neighbor contributions) calculated by Nicholson and Burns[7] are lower than our values by 24 and 8.5% for tetrahedral and octahedral sites, respectively. The results of Nicholson and Burns seem to be in error, especially in the case of the field gradient at tetrahedral sites since they obtained their values by performing the sums from the ions within a sphere of $R=5a$ by a direct lattice summation method[13] without forming any neutral groups, with the result that their sums are suspected to be less convergent. We have checked this by repeating the calculations using their method.[14]

TABLE I. The electric-field-gradient components and the theoretical and experimental values of the quadrupole coupling constants eQq, where q is the resultant electric field gradient, for the tetrahedral and octahedral Fe sites in yttrium iron garnet. Primes are used to denote the results without shielding factors. Field gradients are in units of 10^{14} esu whereas the coupling constants are in MHz.

	Tetrahedral site	Octahedral site
q_l'	−15.1539	−11.6990
q_{nl}'	1.9384	1.5084
q_d'	−0.1179	−0.0697
q_{dB}'	−6.0909	−6.0819
q_n'	4.7354	4.6785
q_{RL}'	0.9562	0.2629
q	−14.2315	−19.2001
eQq (theor)	−18.6 ± 1.5	−25.1 ± 2.3
eQq (expt)	−18.1 ± 3.6	−21.8 ± 4.4

Next, taking the same values of the shielding factors as in Ref. 1, namely, $1-R=0.68$[15] and $1-\gamma_\infty=10.14$,[16] we obtain the total electric field gradient (in units of 10^{14} esu), $q=-14.23$ for tetrahedral Fe sites and $q=-19.20$ for octahedral Fe sites (Table I). The quadrupole coupling constants eQq for the two sites may now be calculated assuming our previous value[1] of $Q(Fe^{57m})=0.18$ b. The calculated results for the two sites (in MHz) are −18.6 (tetrahedral) and −25.1 (octahedral) which are in excellent agreement with the corresponding experimental values,[6,17] −18.1

±3.6 and −21.8±4.4 (Table I). It has been argued in Ref. 1 that $1-R$ and $1-\gamma_\infty$ suffer from some uncertainties in their values. Taking these into account one may write finally the theoretical values of eQq as −18.6±1.5 (tetrahedral) and −25.1 ±2.3 (octahedral). These may be compared with the previously calculated coupling constants (believed to be in error as discussed above), −7 and −17 MHz for tetrahedral and octahedral sites, respectively, calculated by Nicholson and Burns[7] using a monopole approximation, and $Q(\mathrm{Fe}^{57m}) = 0.20$ b.

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Shape of the Island of Superheavy Nuclei*

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On the basis of the Strutinsky shell-correction method applied to realistic diffuse-surface potentials we have calculated the shape of the island of superheavy nuclei. With respect to spontaneous fission, the island is a mountain ridge extending from 114 protons to about 124 protons. The descent from the mountain down to the sea of instability is rather gentle for decreasing neutron numbers below 184, but is more rapid on the other three sides.

In attempts to produce superheavy nuclei near the predicted closed shells at 114 protons and 184 neutrons, it is important to know the stability of these nuclei with respect to their various modes of decay. Because their stability is associated with shell closures, the size and shape of the island of superheavy nuclei depends strongly upon the single-particle potential felt by neutrons and protons near the Fermi surface. In practice this potential must be extrapolated from regions of known nuclei. We have therefore concentrated on techniques that permit more accurate extrapolations, both to the large deformations encountered in fission and to new regions of nuclei, in order to identify more clearly the extent of the island, especially with respect to spontaneous fission.

With this basic purpose in mind, we generate the spin-independent part of the single-particle potential by folding an effective two-nucleon inter-