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Theory of Nuclear Quadrupole Interaction in Nontransition Metals—Magnesium*

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A theoretical investigation of various electronic contributions to the electric field gradient in hcp magnesium has been carried out. The dominant contribution comes from the anisotropic filling of the \bar{k} space and is therefore a Fermi-volume effect. In contrast, the contribution associated with the distortion of the Fermi surface by the $l=2$ component of the lattice potential is found to be extremely small. The total electronic contribution is $0.0046e\alpha_0^3$ and anti-shields the lattice contribution of $0.0018e\alpha_0^3$.

I. INTRODUCTION

The nature of crystalline fields in noncubic metals is of considerable experimental and theoretical interest. For example, the nuclear quadrupole interaction¹ depends upon the electric field gradient (EFG) at the nucleus and its study provides information about the $l=2$ component of the crystalline

field. Furthermore, spin-resonance studies² of rare-earth impurities in noncubic metals provide valuable information about the nature of the crystalline fields in these metals.

In the present paper we investigate the nature of the $l=2$ component of the crystalline field by analyzing the electronic and lattice contributions to the EFG in magnesium. In contrast to other hyperfine

properties,^{1,3} the EFG derives contributions directly from the electrons^{1,4-6} as well as the ionic charges in the lattice. The lattice contribution q_{latt} to the EFG can be evaluated quite accurately^{4,7} and one can then indirectly obtain the electronic contribution q_{el} by subtracting q_{latt} from the experimentally obtained total field gradient q . However, a general theoretical understanding of the origin of q_{el} is still lacking although two notable attempts^{5,6} have been made. One of these studies⁶ was in the semimetal antimony where the smallness of the Fermi surface made the quantitative evaluation of q_{el} from all the electrons in the occupied \vec{k} space particularly simple, by using a Wannier representation for the electronic wave functions. The electronic contribution for this semimetal was found to be a factor of 4 larger and of the same sign (antishielding) as q_{latt} . This contribution, since it arises from the anisotropic filling of \vec{k} space, can be referred to as a Fermi-volume effect. The other investigation,⁵ which proposed a rather interesting mechanism contributing to q_{el} , has been carried out on transition metals and their compounds. For these systems, it was shown that a sizable contribution, again several times larger than q_{latt} , but of opposite sign (shielding), arose from the electrons near the Fermi surface, through the distortion of the latter by the $l=2$ components of the lattice potential.⁸ It is not clear at the present time under what general conditions one of these mechanisms is more important than the other. Another point of interest is that while the sign of q_{el} due to the WGY mechanism is expected to represent a shielding effect, a similar unequivocal statement cannot be made about the Fermi-volume contribution which, for Sb, is an antishielding effect. This is an important question because of the continuing interest⁹⁻¹² in the experimental study of nuclear quadrupole interaction in metals and the fact that the sign of q is becoming available in an increasing number of cases^{10,11} through various experimental techniques.

The present work, representing a first-principles evaluation of the field gradient in metals, is an attempt at answering the questions just raised through a quantitative study of q_{el} in magnesium. The choice of magnesium was dictated by two considerations. First, a fairly detailed understanding of its energy bands as well as hyperfine properties is currently available.^{13,14} Second, it is a metal that is somewhat intermediate between the two extremes represented by antimony and the transition metals with respect to the density of states at the Fermi surface which is directly involved in the WGY mechanism.⁵

In Sec. II we briefly outline the basic equations to obtain q_{el} and q_{latt} . The procedures to obtain the electronic wave functions and the effect of crys-

tal symmetry on contributions to q_{el} from different bands are given in Sec. III. Finally, in Sec. IV, we present the results of our numerical calculation and discuss the relative importance of various contributions to the EFG.

II. BASIC THEORY

The electronic contribution to q , namely, q_{el} is given by

$$q_{\text{el}} = \int \rho_c(\vec{r}) [(3 \cos^2 \theta - 1)/r^3] d\vec{r}, \quad (1)$$

where the nucleus under study is placed at the origin. We will evaluate q_{el} in units of $-e$, the electronic charge. $\rho_c(\vec{r})$ is the total conduction-electron charge density at the point \vec{r} ,

$$\rho_c(\vec{r}) = 2 \sum_{n\vec{k}} |\psi_{n\vec{k}}(\vec{r})|^2, \quad (2)$$

the sum on $n\vec{k}$ being over the occupied states only, n being the band index, and the factor 2 coming from the summation over the spin states. In the present work, the wave functions $\psi_{n\vec{k}}(\vec{r})$ are linear combinations of orthogonalized-plane-wave (OPW) functions, for the calculation of which Falicov's crystal potential¹³ was utilized. It should be noted that this potential does not include the $l=2$ and higher components, the influence of which on q_{el} is incorporated through the WGY mechanism.

In an earlier calculation¹⁴ we had observed that the wave functions obtained by using Falicov's crystal potential and the OPW procedure gave a value of the Knight shift (K_s) which was about 50% of the experimental value. On the other hand, wave functions obtained by a pseudopotential method and using the pseudopotential parameters of Kimball, Stark, and Mueller¹⁵ gave excellent agreement with the experimental value of K_s . It therefore appears that the OPW procedure underestimates the s character of the wave function of the Fermi-surface electrons, particularly their contributions to the spin density at the nucleus. In spite of this limitation of the OPW procedure, we have utilized it to calculate q_{el} for the following two reasons: (i) The pseudopotential parameters were obtained for electrons at the Fermi surface and therefore are inappropriate for off-shell energy eigenvalues and eigenvectors. Since for q_{el} we need the wave functions for the entire occupied \vec{k} space and not just those for the Fermi surface alone, the pseudopotential parameters are inadequate. (ii) In contrast to K_s , which requires the knowledge of the wave function at a point in \vec{r} space, i. e., at the nucleus, the EFG involves an integration over all \vec{r} values and should therefore be less sensitive to the value of the wave function at a single point in \vec{r} space.

Since $\rho_c(\vec{r})$ is a periodic function, one can write

$$\rho_c(\vec{r}) = \sum_{\nu} \rho_c(\vec{r} - \vec{R}_{\nu}). \quad (3)$$

It is convenient to separate the contribution from $\rho_c(\vec{r})$ into two parts, $\hat{\rho}_c(\vec{r})$ referring to the electronic charge density inside the cell containing the nucleus and $\sum_{\nu \neq 0} \hat{\rho}_c(\vec{r} - \vec{R}_\nu)$ from the other cells. The contribution to q_{el} from the first part of the electronic density, namely, $q_{el,1}$, has been obtained using Eq. (1) and calculated wave functions at 5400 \vec{k} points in the first Brillouin zone. The second contribution arising from the electronic charges in the other cells can also be obtained directly using Eq. (1). This contribution is best expressed⁴ as a fraction of the lattice contribution q_{latt} . In magnesium, this contribution is found to be less than 10% of

q_{latt} . The latter requires the replacement of the integration in Eq. (1) by a summation^{4,7} over the ionic charges at the lattice sites. For this contribution, the polarization of the core electrons surrounding the nucleus of Mg^{++} ion, due to q_{latt} , has to be included through a Sternheimer antishielding factor¹⁶ $(1 - \gamma_\infty)$. Thus q_{latt} is related to q_{ion} , the electric field gradient at the nucleus⁴ due to an array of divalent positive ions, by the relation

$$q_{latt} = q_{ion} (1 - \gamma_\infty). \quad (4)$$

The third contribution to q_{el} , $q_{el,3}$, is given by⁵

$$q_{el,3} = q_{WGY} = -2e^2 q_{ion} g(E_F) [\langle \langle \psi_{kF} | r^2 (3 \cos^2 \theta - 1) | \psi_{kF} \rangle \langle \psi_{kF} | r^{-3} (3 \cos^2 \theta - 1) | \psi_{kF} \rangle - \langle \langle \psi_{kF} | r^2 (3 \cos^2 \theta - 1) \times | \psi_{kF} \rangle \rangle \langle \langle \psi_{kF} | r^{-3} (3 \cos^2 \theta - 1) | \psi_{kF} \rangle \rangle], \quad (5)$$

where $\langle A \rangle$ is the expectation value of the operator A over an electronic state at the Fermi surface and $\langle \langle A \rangle \rangle$ refers to the average of the matrix element $\langle A \rangle$ over the Fermi surface. It should be noted that in Eq. (5) there is a coherence effect in the sense that, although the angular part of $\langle A \rangle$ can have different signs for different points on the Fermi surface, that of the product $\langle A \rangle \langle B \rangle$ always has the same sign. Further, the first term of the form $\langle \langle A \rangle \langle B \rangle \rangle$ in the square brackets of Eq. (5) is finite even for a spherical Fermi surface (in the absence of the effect of the $l=2$ component of the potential). The second term, however, vanishes for this case but is finite when the Fermi surface is nonspherical and can give an opposing contribution to the first term.

III. CALCULATION

Contributions from different \vec{k} points inside the first Brillouin zone have been evaluated for all the occupied bands. The electronic wave function for a state \vec{k} and band index n can be written in OPW representation as

$$\psi_{n\vec{k}}(\vec{r}) = \sum_{\vec{K}} C_n(\vec{k} + \vec{K}) \left(\chi_{\vec{k}+\vec{K}} - \sum_t \langle \phi_t | \chi_{\vec{k}+\vec{K}} \rangle \phi_t \right), \quad (6)$$

where $\chi_{\vec{k}+\vec{K}}$ is a properly normalized plane wave and ϕ_t are the core wave functions to which the plane waves are orthogonalized. $\langle \phi_t | \chi_{\vec{k}+\vec{K}} \rangle$ are the orthogonalization parameters. The contribution from each state $n\vec{k}$ is separated into plane-wave and core contributions, the former arising from only the plane-wave components of the OPW functions and the latter referring to terms in the integrand in Eq. (1) involving products of core functions or of plane waves and core functions. The core contributions are further subdivided into p - p and s - d contributions. The p - p -type core contribution is

seen to dominate for each band since the core components of the OPW functions involve the $2p$ wave function of the Mg^{++} ions through orthogonalization. For the s - d -type contribution, on the other hand, the d component of the wave function arises from the plane waves only and involves terms of the form $j_2(kr)$ which have much less density near the nucleus than an atomiclike function. From Table I we see that the plane-wave and s - d components of $q_{el,1}$ are comparable. To understand the signs of the contributions from the various bands, it is helpful to examine the \vec{k} dependence of $q_{el,1}$. Figure 1 shows the \vec{k} dependence of $q_{el,1}$ for the first and second bands which make the leading contributions to $q_{el,1}$. [Note that we have plotted $q_{el,1}$ from Eq. (1), which does not include the factor $-e$, the negative charge of the electron. The actual field gradient should, however, include this negative sign.] The \vec{k} dependence of $q_{el,1}$ in Fig. 1 can be explained from a consideration of the angular character of the conduction-electron wave functions as expected from symmetry arguments. For example, starting from Γ_1^* (s -like) point, where $q_{el,1}$ is expected to vanish, if one moves along the Δ axis to A_1 , the first band has Δ_1 (p_x -like) symmetry and therefore leads to a positive $q_{el,1}$. The second band has Δ_2 (also p_x -like) symmetry, but

TABLE I. Contributions to $q_{el,1}$ from individual bands in magnesium (in units of $-ea_0^3$).

Band	Plane wave	pp	sd	Total
1	-0.003 40	-0.054 63	-0.000 88	-0.058 91
2	0.004 11	0.052 31	0.000 57	0.056 99
3	-0.001 25	-0.004 09	0.000 54	-0.004 80
4	0.000 32	0.001 91	-0.000 08	0.002 15

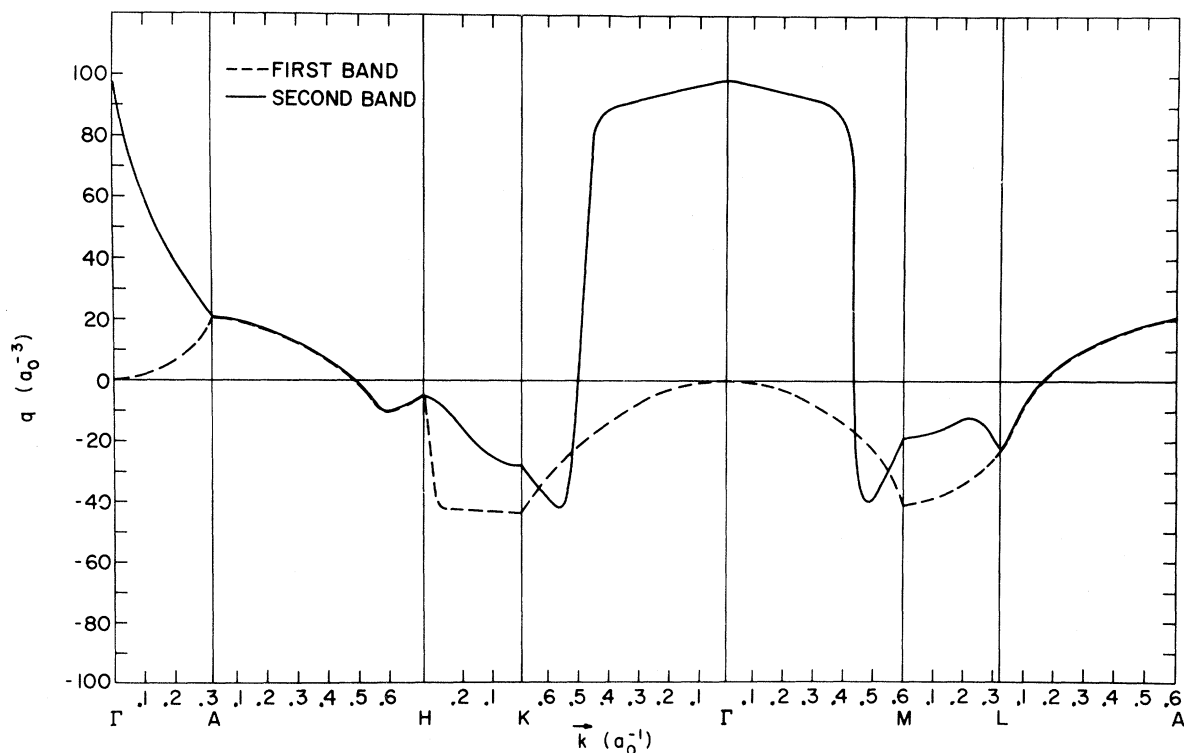


FIG. 1. Contributions to $q_{e1,1}$ as a function of \vec{k} along different symmetry directions. The factor $-e$ is not included and the scale is arbitrary up to a constant multiplicative factor.

since it connects Γ_3^* and A_1 , both involving p_x character, $q_{e1,1}$ is also positive but much larger than the contribution from the first Δ_1 band. A similar interesting situation occurs along the ΓK direction. The first band has T_1 symmetry (s - and p_x - p_y -like) and $q_{e1,1}$ is negative. The second band starting from Γ_3^* has T_2 (p_x -like) symmetry leading to a positive $q_{e1,1}$. In the neighborhood of $|\vec{k}| = 0.5a_0^{-1}$, $|\vec{k}|$ being the length from Γ along the ΓK line, the T_2 band leaves the Fermi surface and $q_{e1,1}$ falls to zero. However, near the K point the second band has T_4 symmetry and therefore $q_{e1,1}$ is negative. The sharp drop in $q_{e1,1}$ from the second band in Fig. 1 at $|\vec{k}| = 0.5a_0^{-1}$ on the ΓK line is thus the result of the fact that the second band in this direction consists of two bands of different symmetry. Thus, the signs of the total $q_{e1,1}$ from the various bands are a result of the combination of contributions of opposing signs from various points in \vec{k} space. In addition, there appears to be a substantial cancellation between the contributions from the various bands. These cancellation effects emphasize the need for a careful scanning of the \vec{k} space and accurate evaluation of the contributions from each point in \vec{k} space.

IV. RESULTS AND DISCUSSION

The lattice contribution to q has been evaluated earlier for magnesium and we only quote the result.

Using a value 4.2 for the Sternheimer antishielding for factor¹⁶ $(1 - \gamma_\infty)$, we have

$$q_{\text{latt}} = 0.0018 e a_0^{-3}. \quad (7)$$

The electronic contribution $q_{e1,2}$ from noncentral cell charge distribution was estimated to be

$$q_{e1,2} = 0.0002 e a_0^{-3}. \quad (8)$$

The major electronic contribution that we have calculated using OPW functions is

$$q_{e1,1} = 0.0046 e a_0^{-3}. \quad (9)$$

As we see, $q_{e1,1}$ is more than a factor of 2 larger than the lattice contribution in Eq. (7).

For the WGY contributions,⁵ one needs the values of the two terms in the square brackets of Eq. (5), both of which require an averaging over the Fermi surface. This averaging involves all four segments¹³ of the Fermi surface, namely, the lens, cigars, butterflies, and monster. For the first term, the signs of the contributions from all four segments are found to be the same (positive), while for the second term, there is substantial cancellation, the contributions from the cigars, butterflies, and monster having positive sign and the lens a negative sign. It was pointed out before that the second term vanishes for a spherical Fermi surface. For magnesium, we find that even after cancellation between various segments of the Fer-

mi surface, the second term is about 40% of the first term. The net values of the two terms in the square brackets of Eq. (5) are, respectively, $5.23a_0^{-1}$ and $2.14a_0^{-1}$, leading to a value of $3.09a_0^{-1}$ which results in

$$q_{\text{WGY}} = -0.0001ea_0^{-3}. \quad (10)$$

This is an order of magnitude smaller than $q_{e1,1}$. On combining the three contributions to q , one gets

$$q_{\text{total}} = 0.0065ea_0^{-3}. \quad (11)$$

This compares very well with the value $q_{\text{expt}} = 0.0063ea_0^{-3}$ that one obtains from the experimental value¹⁷ of e^2qQ for magnesium and the nuclear quadrupole moment¹⁸ for Mg^{25} derived from atomic quadrupole-coupling data in the excited $3s3p(^3P)$ state.

The relative smallness of q_{WGY} for magnesium, where the density of states at the Fermi energy, dn/dE_{F} , is sizable, in contrast to the semimetal antimony¹⁹ for which the density of states is negligible, indicates that for the WGY mechanism to be dominant or comparable to the Fermi-volume mechanism one requires a very large density of states accompanied with substantial non- s ($l \neq 0$) character at the Fermi surface. The transition metals with d bands near the Fermi surface for which the WGY mechanism⁵ was first developed appear to be the most appropriate ones in this respect. However, since in magnesium our calculations show that the Fermi-volume effect is about two orders of magnitude larger than the contribution from the WGY mechanism, it is quite possible that the Fermi-volume contribution from the d -band electrons in transition metals can be comparable to that contributed via the WGY mechanism. This question can be answered by actual calculations in transition metals. In this connection, in rhenium metal, which has $5d$ -band electrons, there seems to be evidence¹¹ that a contribution comparable to the estimated WGY contribution is needed to explain the experimental result.

In comparing the theoretical value of q_{total} for magnesium with experiment, too much significance should not be attached to the near-exact agreement between theory and experiment. The theoretical

value has an uncertainty of about 5% from considerations of convergence of the Fermi-volume contribution with respect to the number of OPW functions occurring in the wave function. In addition, for $q_{e1,1}$, we have not used any antishielding factor because it is expected to be much smaller than $(1 - \gamma_{\infty})$ and more in the nature of an atomic antishielding factor¹⁶ $(1 - R)$. From atomic calculation²⁰ of R one finds it to be of the order of 0.1 and hence the $(1 - R)$ factor will not change the band contributions appreciably. One might worry about the differences in $(1 - R)$ for different bands, particularly for the two lowest bands. However, our analysis of the wave functions indicates that both bands are made up of $3s$ and $3p$ characters. They differ in the relative mixing of these two characters, as well as in the nature of their angular distributions, namely, the relative amounts of $3p_x$, $3p_y$, and $3p_z$ characters. Since R depends on the interaction between the spherical $1s^2$, $2s^2$, $2p^6$ core and the $3p$ radial density, independent of the angular character of the latter, we do not expect $(1 - R)$ to be significantly different for the two bands.

As far as the experimental result is concerned, there is also some uncertainty due to the influence of neglected many-body effects on the atomic field gradient in the $3s3p(^3P)$ state which was used to derive the quadrupole moment Q of Mg^{25} , which in turn was used to obtain q_{expt} in the metal from the experimental value of e^2qQ .

V. CONCLUSION

In summary, the results of our calculation have indicated that a first-principles evaluation of q using actual wave functions in the metal does produce reasonable agreement with experiment in magnesium. The nature of the various contributions to q indicates that the Fermi-volume contribution $q_{e1,1}$ is the main contributor in nontransition metals and can have either a positive or negative sign. The WGY Fermi-surface mechanism⁵ is expected to be significant mainly in transition metals with a large density of states at the Fermi surface, but here also a quantitative evaluation of $q_{e1,1}$ is desirable, as it may well be comparable to q_{WGY} .

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