# Theoretical Study of the Indirect Quadrupole-Quadrupole Interactions in Metals and Alloys*

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Z. Naturforsch. **45a**, 380–384 (1990); received August 23, 1989; in revised form December 1, 1989

The indirect multipole interactions of nuclei and impurity paramagnetic ions in metals and alloys via conduction electrons are investigated by means of the dielectric function method. The Hamiltonian of the indirect quadrupole-quadrupole interaction of impurity paramagnetic ions and nuclei is constructed selfconsistently, taking into account the exchange interactions and correlations of the conduction electrons as well as the antishielding effects. It is shown that the energy of these indirect quadrupole interactions of the nuclei and the paramagnetic ions decreases with the distance as $R^{-3}$, oscillating with a period which is determined by the wave vector on the Fermi surface and the distance $R$. The influence of these indirect quadrupole-quadrupole interactions on the width and shape of the NMR lines is studied.

*Key words:* Quadrupole, Interactions, Nuclei, Metals, Resonance.

## 1. Introduction

A crucial factor for the interpretation of experimental results obtained by NMR and NQR techniques is a proper treatment of all contributions to the electric field gradient (EFG) at the nuclei and of all interactions that can contribute to the NMR and NQR parameters, direct as well as indirect via conduction electrons nuclear spin-spin interactions [1–7]. Note that experimental evidence was obtained in [8–11] for the necessity to take into consideration multipolar pair interactions to explain the temperature variation of the EFG at impurity sites in rare-earth metals and alloys, elastic constant, parastriction and magnetic susceptibility of rare-earth intermetallic compounds, and the temperature variation of the anisotropy of the magnetic susceptibility of rare-earth metals. The direct electric quadrupole-quadrupole interaction is small and of opposite sign [8–11].

In the present work we investigate the indirect quadrupole-quadrupole interactions between nuclei with spin $I \geqq 1$ as well as between nuclei and impurity paramagnetic ions in metals and alloys which arise because of the perturbation of the charge density of the conduction electrons by the electric quadrupole moments of the nuclei and the ions.

We note that Kessel [12] has calculated the indirect quadrupole interactions between nuclei in metals via conduction electrons only to the second order in the interaction between the nuclear quadrupole moment and the EFG formed by a conduction electron, using Bardeen's approximation for the conduction electron wave function [13]. Besides, the many body effect on the nuclear quadrupolar interaction in metals and the appropriate contributions to the antishielding factors [14] have not been taken into account in [12].

## 2. Calculation of the Induced Charge Density

We use the dielectric function method of Pines [15] to calculate the induced charge density of conduction electrons due to the electric quadrupole moment of the impurity paramagnetic ion (nucleus) at the origin. According to [15], in the selfconsistent case, the expression for the Fourier component of the induced charge density $n(\boldsymbol{k})$ can be written in the form

$$n(\boldsymbol{k}) = -\{[\varepsilon(\boldsymbol{k})-1]\, k^2/4\pi\, \varepsilon(\boldsymbol{k})\}\, \Phi(\boldsymbol{k}), \qquad (1)$$

where $\varepsilon(\boldsymbol{k})$ is the dielectric function of the conduction electrons and $\Phi(\boldsymbol{k})$ the Fourier component of the external potential caused by the electric quadrupole moment of the paramagnetic ion (nucleus):

$$\Phi(\boldsymbol{k}) = \int \Phi(\boldsymbol{r}) \exp(i\,\boldsymbol{k}\,\boldsymbol{r})\, \mathrm{d}\boldsymbol{r}, \qquad (2)$$

$$\Phi(\boldsymbol{r}) = (4\pi/5)^{1/2} \sum_{m=-2}^{2} Q_{2,m}\, Y^*(\Theta_r, \varphi_r)\, r^{-3}\, \Gamma. \qquad (3)$$

* Presented at the Xth International Symposium on Nuclear Quadrupole Resonance Spectroscopy, Takayama, Japan, August 22–26, 1989.

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Here $\Theta_r$, $\varphi_r$ are the polar angles of the radius-vector $\boldsymbol{r}$, $Q_{2,m}$ is the component of the electric quadrupole moment of the impurity ion (nucleus) and $\Gamma$ the antishielding factor [14] ($\Gamma=1-R'$ for the impurity paramagnetic ion, $\Gamma=1-\gamma_\infty$ for the nucleus).

On taking the exchange and correlation effects of the conduction electrons into consideration and using the plane wave approximation for the conduction electron wave functions, the dielectric function $\varepsilon(\boldsymbol{k})$ can be expressed in the following form [16]:

$$\varepsilon(\boldsymbol{k})=1+\chi(k)[1-\chi(k)f(k)]^{-1}, \tag{4}$$
$$f(k)=[(k^2/k^2+k_F^2+k_S^2)+(k^2/k_F^2+k_S^2)]/4,$$
$$\chi(k)=k_{FT}^2\{(1/2)+[k_F(1-k^2/4k_F^2)\cdot\ln|(k+2k_F)/(k-2k_F)|/2k]\}/k^2.$$

$k_F$ the wave vector on the Fermi surface, $k_S$ the inverse screening radius, $k_{FT}=(6\pi N e^2/E_F)^{1/2}$ the inverse Tomas-Fermi screening radius, $N$ the concentration of conduction electrons and $-e$ the electronic charge. We expand the plane wave in spherical functions:

$$e^{i\boldsymbol{k}\boldsymbol{r}}=4\pi\sum_{l=0}^{\infty}i^l j_l(kr)\sum_{m'=-l}^{l}Y_{l,m'}(\Theta_r,\varphi_r)\,Y_{l,m'}^*(\Theta_k,\varphi_k), \tag{5}$$

where the coefficients $j_l(kr)=(\pi/2kr)^{1/2}\,J_{l+1/2}(kr)$ are the spherical Bessel functions and $\Theta_k$, $\varphi_k$ the polar angles of the vector $\boldsymbol{k}$. Due to (1), (2), (3), and (5) and the orthogonality of the spherical functions, the Fourier component of the induced charge density $n(\boldsymbol{k})$ can be written as

$$n(\boldsymbol{k})=(4\pi/5)^{1/2}\{[\varepsilon(k)-1]\,k^2/3\,\varepsilon(k)\}\cdot\sum_{m=-2}^{2}Q_{2,m}\,Y_{2,m}^*(\Theta_k,\varphi_k)\,\Gamma. \tag{6}$$

We perform the inverse Fourier transform of (6) and, having expanded the plane wave $\exp(-i\boldsymbol{k}\boldsymbol{R})$ in spherical functions, integrate over the angle variables of the vector $\boldsymbol{k}$. Then we obtain

$$n(\boldsymbol{R})=-(4\pi/5)^{1/2}\sum_{m=-2}^{2}Q_{2,m}\,Y_{2,m}^*(\Theta_R,\varphi_R)\,\Gamma\cdot\int_0^\infty[(\varepsilon(k)-1)\,k^4 j_2(kR)/6\pi\,\varepsilon(k)]\,dk. \tag{7}$$

We take the singularity of $\chi(k)$ at $k=2k_F$ into account and use the asymptotic form of the Fourier transform of the generalized function [17]. On limiting ourselves to terms inversely proportional to $R^4$ in the expression for the induced charge density of conduction electrons $n(\boldsymbol{R})$, finally, in the limit of large $R$, we obtain the following expression for $n(\boldsymbol{R})$

$$n(\boldsymbol{R})=\{[-F\cos(2k_F R)/R^3]+G[\ln(k_F R)+g]\sin(2k_F R)/R^4\}\,\Gamma\cdot(4\pi/5)^{1/2}\left\{\sum_{m=-2}^{2}Q_{2,m}\,Y_{2,m}^*(\Theta_R,\varphi_R)\right\}\Big/6\pi, \tag{8}$$

$$F=16\pi p\,k_F^2/(4+pa)^2,\quad a=1-f(2k_F),\quad p=k_{FT}^2/2k_F^2,$$
$$G=8\pi p^2 a\,k_F/(4+pa)^3,\ g=\gamma-\{3(4+pa)/pa\}-3/2,$$
$$\gamma=0{,}5772.$$

### 3. The Components of the Electric Field Gradient

According to [10, 18], the component $B_{2,\xi}^{ij}$ of the EFG at the nucleus located at the lattice site $i$, due to the electronic charge density, perturbed by the electric quadrupole moment of the $j$-th impurity paramagnetic ion ($j$-th nucleus) at the origin, is given by

$$B_{2,\xi}^{ij}=(4\pi/5)^{1/2}\int d\boldsymbol{r}'\,n(\boldsymbol{r}'-\boldsymbol{R}_{ij})\,Y_{2,\xi}(\Theta',\varphi')\,(r')^{-3}, \tag{9}$$

where $\boldsymbol{r}'$ is the radius-vector of an electron relative to the lattice site $i$, $\boldsymbol{R}_{ij}$ the radius-vector directed from the lattice site $i$ to the origin and $\Theta'$, $\varphi'$ are the polar angles of the radius-vector $\boldsymbol{r}'$. After inserting (8) into (9), we get under the integral two spherical functions from the two centers 0 and $i$. To calculate $B_{2,\xi}^{ij}$, we transform the two-center integral to the one-center integral (to the center located at the lattice site $i$) with the help of the relation [19]

$$r^l\,Y_{l,m}(\Theta,\varphi)=\sum_{l_1 m_1}\sum_{l_2 m_2}(2l+1)^{1/2}(2l+1)!!\cdot(4\pi)^{1/2}(-1)^{l_1-m_1+l_2-m_2}\begin{pmatrix}l_1 & l & l_2\\ -m_1 & m & -m_2\end{pmatrix}\cdot(l_1\|C^l\|l_2)\,r_1^{l_1}r_2^{l_2}\,Y_{l_1m_1}(\Theta_1,\varphi_1)\,Y_{l_2m_2}(\Theta_2,\varphi_2)\cdot[(2l_1+1)!!\,(2l_2+1)!!]^{-1}, \tag{10}$$

where round brackets ( ) define $3j$-symbols, $(l_1\|C^l\|l_2)$ the standard submatrix element, $\Theta$, $\varphi$ the polar angles of the radius-vector $\boldsymbol{r}$ directed from the center 0 to the point $A$, $\Theta_1$, $\varphi_1$ are the polar angles of the vector $\boldsymbol{r}_1$ directed from the center 1 to the point $A$ *and* $\Theta_2$, $\varphi_2$ the polar angles of the vector $\boldsymbol{r}_2$ directed from the center 2 to the center 1. The summation is over $l_1$ and $l_2$, which satisfy the relation $l_1+l_2=l$. Following [20], we suppose that the main contribution to the components of the EFG is due to the region with small $r'$ and restrict ourselves to the contribution from a region inside the sphere with radius $R_{ij}/2$ with the center at the lattice site $i$, for which we suppose that $r'\ll R_{ij}$. We also suppose that the $Z$ axis is directed along the vector $\boldsymbol{R}_{ij}$.

Inserting (8) into (9) and using (10), we obtain

$$B^{ij}_{2,\xi}=(5)^{1/2}\sum_{m=-2}^{2}(-1)^m Q^j_{2,m}$$
$$\cdot\sum_{l_1 m_1}\sum_{l_2}(-1)^{l_1-m_1+l_2}(2l_2+1)^{1/2}[(2l_1+1)!!(2l_2+1)!!]^{-1}$$
$$\cdot\begin{pmatrix} l_1 & 2 & l_2\\ -m_1 & -m & 0\end{pmatrix}(l_1\|C^2\|l_2)$$
$$\cdot\{\int \mathrm{d}\boldsymbol{r}'(r')^{l_1-3}\,Y_{l_1 m_1}(\Theta',\varphi')\,Y_{2,\xi}(\Theta',\varphi')$$
$$\cdot[-R_{ij}^{l_2-5}(e^{2ik_F(R_{ij}-r'\cos\Theta')}+e^{-2ik_F(R_{ij}-r'\cos\Theta')})$$
$$-i R_{ij}\,G\,[\ln(k_F R_{ij})+g]$$
$$\cdot(e^{2ik_F(R_{ij}-r'\cos\Theta')}-e^{-2ik_F(R_{ij}-r'\cos\Theta')})]\}. \quad (11)$$

Here $Q^j_{2,m}$ is the component of the electric quadrupole moment of the $j$-th impurity paramagnetic ion ($j$-th nucleus). The summation is over $l_1$ and $l_2$, which satisfy the relation $l_1+l_2=2$. Using the expansion of the plane wave (5), we obtain

$$e^{2ik_F r'\cos\Theta'}=4\pi\sum_{l=0}^{\infty} i^l j_l(2k_F r')[(2l+1)/4\pi]^{1/2}\,Y_{l,0}(\Theta',\varphi'). \quad (12)$$

Inserting (12) in (11), we perform the integration over the angle variables of the vector $\boldsymbol{r}'$. Then we obtain

$$\int Y_{l_1 m_1}(\Theta',\varphi')\,Y_{2,\xi}(\Theta',\varphi')\,Y_{l,0}(\Theta',\varphi')\,\mathrm{d}\Omega' \quad (13)$$
$$=[(2l_1+1)(2l+1)\,5/4\pi]^{1/2}\begin{pmatrix} l_1 & 2 & l\\ 0 & 0 & 0\end{pmatrix}\begin{pmatrix} l_1 & 2 & l\\ m_1 & q & 0\end{pmatrix}.$$

Taking into account the properties of $3j$-symbols and limiting ourselves to terms proportional to $R_{ij}^{-5}\ln(k_F R_{ij})$, we finally get the following expression for $B^{ij}_{2,\xi}$

$$B^{ij}_{2,\xi}=R_{ij}^{-3}\{Q^j_{2,\xi}[F S_\xi(2k_F R_{ij}) + G T_\xi(2k_F R_{ij})/R_{ij}]\,\Gamma_i\Gamma_j\}, \quad (14)$$

where

$$S_0(X)=(2\cos X/9) -[(88\cos X-488\cos X\cos(X/2))/105X^2] -[16\sin X\sin(X/2)/3X^2],$$
$$S_{\pm1}(X)=(4\sin X/3X) -[(8\cos X+32\cos X\cos(X/2))/105X^2] -[16\sin X\sin(X/2)/5X^2],$$
$$S_{\pm2}(X)=(-50\cos X/21X^2) -4\cos X\cos(X/2)/35X^2,$$
$$T_0(X)=\{-2\sin X[\ln(X/2)+\gamma-3/2]/9\} +[88\sin X\ln(X/2)/35X^2] +[68\sin X\cos(X/2)\ln(X/2)/35X^2],$$
$$T_{\pm1}(X)=\{-8\cos X[\ln(X/2)+\gamma-3/2]/3X\} +8\sin X\ln(X/2)/105X^2 +32\sin X\cos(X/2)\ln(X/2)/105X^2,$$
$$T_{\pm2}(X)=[248\sin X\ln(X/2)/105X^2] +[4\sin X\cos(X/2)\ln(X/2)/35X^2].$$

## 4. The Hamiltonian of the Indirect Quadrupole-Quadrupole Interaction

The Hamiltonian of the indirect quadrupole-quadrupole interaction via the conduction electrons between the $j$-th impurity paramagnetic ion ($j$-th nucleus) and $i$-th nucleus for a system of coordinates with the $Z$ axis directed along the vector $\boldsymbol{R}_{ij}$ has the form

$$H^{ij}_{Q-Q}=\sum_{\xi=-2}^{2}(-1)^\xi B^{ij}_{2,-\xi}Q^i_{2,\xi} =\sum_{\xi=-2}^{2}(-1)^\xi V^{|\xi|}_{ij}Q^i_{2,\xi}Q^j_{2,-\xi}, \quad (15)$$

where

$$V^{|\xi|}_{ij}=R_{ij}^{-3}\{F S_\xi(2k_F R_{ij})+G R_{ij}^{-1}T_\xi(2k_F R_{ij})\}\,\Gamma_i\Gamma_j. \quad (16)$$

According to [18], the operators of the components of the electric quadrupole moment of the $j$-th impurity rare-earth ion with the total angular momentum $\boldsymbol{J}_j$ can be expressed in the form

$$Q^j_{2,0}=-e\langle J\|\alpha\|J\rangle\langle r_f^2\rangle[3J_{jz}^2+J(J+1)]/2, \quad (17\text{a})$$
$$Q^j_{2,\pm1}=-e\langle J\|\alpha\|J\rangle\langle r_f^2\rangle(3/8)^{1/2}[J_{jz}J_{j\pm}+J_{j\pm}J_{jz}], \quad (17\text{b})$$
$$Q^j_{2,\pm2}=-e\langle J\|\alpha\|J\rangle\langle r_f^2\rangle(3/8)^{1/2}J_{j\pm}^2. \quad (17\text{c})$$

Here $\langle r_f^2\rangle$ is the average square of the $4f$-electron radius and $\langle J\|\alpha\|J\rangle$ the numerical Elliott-Stevens coefficient [18]. The operators of the components of the electric quadrupole moment of the $i$-th nucleus have the form [10, 18]

$$Q^i_{2,0}=\{eQ/2I(2I-1)\}\{3I_{iz}^2-I(I+1)\}, \quad (18\text{a})$$
$$Q^i_{2,\pm1}=\mp\{eQ/2I(2I-1)\}(3/2)^{1/2}(I_{i\pm}I_{iz}+I_{iz}I_{i\pm}), \quad (18\text{b})$$
$$Q^i_{2,\pm2}=\{eQ/2I(2I-1)\}(3/2)^{1/2}I_{i\pm}^2. \quad (18\text{c})$$

$I_i$ is the nuclear spin moment at the lattice site $i$.

In the coordinate system $\tilde{X}, \tilde{Y}, \tilde{Z}$, in which the angle between the $\tilde{Z}$ axis and the vector $\boldsymbol{R}_{ij}$ is $\Theta_{ij}$, the Hamiltonian of the indirect quadrupole-quadrupole interaction can be written as [20]

$$H_{Q-Q} = \sum_{i<j} \sum_{\xi=-2}^{2} W_{ij}^{|\xi|} \tilde{Q}_{2,\xi}^{i} \tilde{Q}_{2,-\xi}^{j}, \tag{19}$$

$$\begin{aligned} W_{ij}^{0} &= (1-3\sin^2\Theta_{ij}/2)\,V_{ij}^{0} \\ &\quad -(3\sin^2 2\Theta_{ij} V_{ij}^{|1|} - 3\sin^4\Theta_{ij} V_{ij}^{|2|})/4, \\ W_{ij}^{|1|} &= -(3\sin^2 2\Theta_{ij} V_{ij}^{0}/8) \\ &\quad +[1-(5\sin^2\Theta_{ij}/2)+2\sin^4\Theta_{ij}]\,V_{ij}^{|1|} \\ &\quad -\sin^2\Theta_{ij}(1-\sin^2\Theta_{ij}/2)\,V_{ij}^{|2|}, \\ W_{ij}^{|2|} &= (3\sin^4\Theta_{ij} V_{ij}^{0}/8) \\ &\quad -\sin^2\Theta_{ij}(1-\sin^2\Theta_{ij}/2)\,V_{ij}^{|1|} \\ &\quad +(1-\sin^2\Theta_{ij}+\sin^4\Theta_{ij}/8)\,V_{ij}^{|2|}. \end{aligned}$$

Here $\tilde{Q}_{2,\xi}^{j}, \tilde{Q}_{2,-\xi}^{i}$ are the operators of the components of the electric quadrupole moment of the $j$-th ion ($j$-th nucleus) and the $i$-th nucleus defined relative to the coordinate system $\tilde{X}, \tilde{Y}, \tilde{Z}$; the summation in (19) is over all pairs of nuclei.

The expressions (15), (16), (19) describe also the indirect quadrupole-quadrupole interactions via conduction electrons of the paramagnetic ion-nuclei, the ground state of which in the electric crystal field is the electronic spin singlet. But the operator $Q_{2,\xi}^{j}$ ($Q_{2,-\xi}^{i}$) in (15), (19) should be changed to the operator of the effective nuclear electric quadrupole moment $\tilde{Q}_{2,\xi}^{\prime j}$ ($\tilde{Q}_{2,-\xi}^{\prime i}$) [21]. The expressions for the components of the effective nuclear quadrupole moments can be obtained using the Nuclear Spin Hamiltonian for the rare-earth ion with singlet ground state [22].

Since the average value of the total angular momentum of the ion $\boldsymbol{J}$ in the singlet ground state is zero, the parameters of the Nuclear Spin Hamiltonian can be calculated in the same way as the parameters of the Spin Hamiltonian [18] of the 3d-ions in the singlet orbital state. That is why we can use well-known formulas of Abragam and Pryce [23], changing in them the spin-orbit constant $\lambda$ to the hyperfine constant $A_S$, the orbital moment $\boldsymbol{L}$ to the total angular momentum $\boldsymbol{J}$ and the electron spin $\boldsymbol{S}$ to the nuclear spin $\boldsymbol{I}$. For axial symmetry of the electric crystal field and arbitrary spin $I$ the components $\tilde{Q}_{2,\xi}^{\prime}$ are [24]

$$\tilde{Q}_{2,0}^{\prime} = [1-(3/2)\sin^2\omega]\,T_{2,0}/4, \tag{20a}$$

$$\tilde{Q}_{2,\pm 1}^{\prime} = \mp(6)^{1/2}\sin 2\omega\, T_{2,0}/4, \tag{20b}$$

$$\tilde{Q}_{2,\pm 2}^{\prime} = (6)^{1/2}\sin^2\omega\, T_{2,0}/4, \tag{20c}$$

where

$$\begin{aligned} T_{2,0} = \{&[3eQ/2I(2I-1)] \\ &+2A_S(\Lambda_{xx}-\Lambda_{yy})/eq\}\,[I_z^2 - I(I+1)/3], \end{aligned} \tag{21}$$

$$\Lambda_{ii} = \sum_{v=0} A_S |\langle 0 \| J_i \| v \rangle|^2/(E_v - E_0), \tag{22}$$

$eq$ is the EFG caused by the asymmetric charge distribution of the paramagnetic ion electrons, by the conduction electrons and by the lattice, $\omega$ is the angle between the crystal $c$-axis and the radius-vector $\boldsymbol{R}_{ij}$, $|0\rangle, |v\rangle$ are the wave functions of the ground and excited states of the rare-earth ion.

For rhombic symmetry of the electric crystal field the components $\tilde{Q}_{2,\xi}^{\prime}$ are [24]

$$\tilde{Q}_{2,0}^{\prime} = [1-(3/2)\sin\psi]\,\tilde{T}_{2,0} + (6)^{1/2}[\tilde{T}_{2,+2}+\tilde{T}_{2,-2}], \tag{23a}$$

$$\begin{aligned} \tilde{Q}_{2,\pm 1}^{\prime} = &-(6)^{1/2}[\sin 2\psi\, \tilde{T}_{2,0}/4] \\ &+[\cos^2(\psi/2)\,\tilde{T}_{2,\pm 2} - \sin^2(\psi/2)\,\tilde{T}_{2,\mp 2}]\sin\psi, \end{aligned} \tag{23b}$$

$$\begin{aligned} \tilde{Q}_{2,\pm 2}^{\prime} = &(6)^{1/2}[\sin^2\psi\, \tilde{T}_{2,0}/4] \\ &+\cos^4(\psi/2)\,\tilde{T}_{2,\pm 2} + \sin^4(\psi/2)\,\tilde{T}_{2,\mp 2}, \end{aligned} \tag{23c}$$

where

$$\begin{aligned} \tilde{T}_{2,0} = \{&[3eQ/2I(2I-1)] \\ &+A_S(\Lambda_{xx}+\Lambda_{yy}-2\Lambda_{zz})/2\}\,[I_z^2 - I(I+1)/3], \end{aligned} \tag{24a}$$

$$\begin{aligned} \tilde{T}_{2,\pm 2} = (3/8)^{1/2}\{&[eQ/2I(2I-1)]\,\eta \\ &+A_S(\Lambda_{yy}-\Lambda_{xx})/2\}\,I_{\pm}^2. \end{aligned} \tag{24b}$$

Here $\psi$ is the angle between the symmetry $Z$ axis of the electric crystal field and the radius-vector $\boldsymbol{R}_{ij}$ and $\eta$ is the asymmetry parameter of the crystal field.

## 5. Contribution of the Indirect Quadrupole-Quadrupole Interaction to the Resonance Linewidth

According to (15), (16), (19), the indirect quadrupole-quadrupole interaction of the impurity paramagnetic ions and the nuclei in metals and alloys ranges farer than the direct quadrupole-quadrupole interaction of the ions and the nuclei. The energy of this indirect multipolar interaction decreases with the distance $R_{ij}$ between the $j$-th paramagnetic ion ($j$-th nucleus) and $i$-th nucleus as $R_{ij}^{-3}$, oscillating with a period which is determined by the value of the wave vector on the Fermi surface and $R_{ij}$.

Contrary to the indirect spin-spin exchange interaction via conduction electrons between identical nuclei, which induces narrowing of the magnetic resonance linewidth, the indirect quadrupole-quadrupole interactions due to the nonisotropic spin part of the Hamiltonian can be considered as an additional source of broadening of the resonance lines. Let us consider the contribution of the indirect nuclear quadrupole-quadrupole interaction via conduction electrons in metals to the NMR linewidth. If the form of the resonance line is close to Gaussian, conclusions about the linewidth can be made, knowing only its second moment. The second moment $M_2$, caused by the indirect quadrupole interaction, is given by [25]

$$h^2 M_2 = [e Q/I(2I-1)]^4 I(I+1)[I(I+1)-3/4]^2 16 \cdot \sum_{j \neq i} \{[2(W_{ij}^0 + 9 W_{ij}^{|1|}/2)^2/3] + 9(W_{ij}^{|1|} + 2 W_{ij}^{|2|})^2 + 135 (W_{ij}^{|1|})^2/2\}/105. \quad (25)$$

The second moment $M_2'$ caused by the nuclear magnetic dipolar interaction is given by [18]

$$h^2 M_2' = (3/5)(\gamma_N \hbar)^4 I(I+1) \sum_j R_{ij}^{-6}, \quad (26)$$

where $\gamma_N$ is the gyromagnetic ratio for the nuclear spins, the average over the angles having been taken. For the NMR linewidth in the crystalline power of $Au^{197}$ ($I=3/2$, $Q=6 \cdot 10^{-24}$ cm$^2$ [26], $E_F=5.49$ eV, $k_F=1.21 \cdot 10^8$ cm$^{-1}$, $k_{FT}=1.73 \cdot 10^8$ cm$^{-1}$ [27], $k_S=k_{FT}$ [16], $\mu=0.1439\,\mu_N$ [6], $\gamma_\infty=-72$ [14]) we obtain $M_2/M_2'=3.74$.

Thus we may conclude that for the crystalline powder of $Au^{197}$ the indirect quadrupole-quadrupole interactions between nuclei make a contribution to the NMR linewidth comparable to the contribution from the magnetic dipolar interaction between nuclei.

Alongside with the indirect spin-spin exchange interaction between the nonidentical nuclei with the atomic number larger than 100 and $I \geqq 1$, additional broadening of the resonance lines may be caused by the indirect nuclear quadrupole-quadrupole interaction if the magnitudes of the quadrupole moments of the nonidentical nuclei and the antishielding factors are sufficiently large [3].

The influence of indirect quadrupole interactions of rare-earth ion-nuclei on the shape and width of magnetic resonance lines on the electron-nuclear levels should increase when the ground state of the ion is the electron spin singlet. According to (22)–(24), the expressions for the components of the effective nuclear electric quadrupole moments contain terms, which depend on the excited states of the paramagnetic ion and reflect the symmetry of the electric crystal field acting on the ion. Due to the large value of the electron magnetic moment of the paramagnetic ion in the excited state compared to the nuclear magnetic moment, the effective nuclear quadrupole moment substantially exceeds the nuclear quadrupole moment. Besides, the antishielding factors in the rare-earth ions are large [14].

*Acknowledgements*

The author is grateful to B. I. Kochelaev for a fruitful discussion of the results and for valuable comments.

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