Structural Disorder and NMR of Quadrupolar Nuclei

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Abstract

Growing computational power in connection with an increasing accuracy of nuclear magnetic resonance (NMR) measurements requires precise models for fitting NMR spectra. The occurrence of structural disorder in the material causes an inaccuracy of NMR signals fitted with standard methods. This article presents the calculation of distribution of the quadrupolar coupling constant and asymmetry parameter of the electric field gradient (EFG) tensor in solids with local disorder. In this work, the calculation was made directly from the disturbance of the initial electric charge system surrounding the quadrupolar nucleus without using an approach based on EFG tensor invariants.

1 Introduction

The precise fitting of powder nuclear magnetic resonance (NMR) spectra of quadrupolar nuclei requires powerful computers. The necessity of integration over all orientation of crystalites gives a spectrum without an analytic representation. In addition to that, the use of the well-known models [1] in connection with a high accuracy of NMR measurements causes a perfect fit not being possible at each attempt [2, 3]. This may be because of many reasons: from some unidentified apparatus errors to an inaccuracy of the physical model. For many compounds, such as glasses with coordination number less or equal to 3 (e.g. boron glasses) [4], nanomaterials [5, 6] and other substances with structural disorder, a similar approach as for powders [1] cannot be used anymore. Random deformations occurring in such materials should be taken into account in high precision measurements.

The basic problem in this situation is to determine a joint distribution of parameters describing quadrupolar interaction. In this work, such a distribution is obtained without using an approach based on electric field gradient (EFG) tensor invariants [7–9]. This approach can be useful for compounds with structural disorder

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2 EFG Tensor

The part of the Hamiltonian corresponding to the nuclear quadrupole interaction can be written as [1, 11]:

$$H_Q = \frac{eQ}{2I(2I-1)\hbar} \mathbf{I} \cdot \mathbf{V} \cdot \mathbf{I},$$

where Q is the nuclear quadrupole moment and $\mathbf{V}$ is the electric field gradient (EFG) tensor with components in the Cartesian coordinates:

$$V_{ik} = \frac{\partial^2 \varphi}{\partial x_i \partial x_k}, \quad (1)$$

where φ is the electric field potential at the nucleus. The EFG tensor is symmetric and traceless, thus it has five independent components. In this article the Cartesian coordinates will be used interchangeably ($x_1 \equiv x$, $x_2 \equiv y$, $x_3 \equiv z$). The components (1) for a discrete charges q_n system can be written as:

$$V_{ik} = \sum_n q_n \left(3x_i^{(n)} x_k^{(n)} - r_n^2 \delta_{ik} \right) r_n^{-5},$$

where $r = \sqrt{x^2 + y^2 + z^2}$. The EFG tensor can be diagonalized by the suitable choice of a coordinate system. Such a system is called the principal axis system (PAS) in which only two components are independent.

The complete definition of the EFG tensor requires five quantities. Instead of V_{ik} components, the other five are used: V_{zz}^{PAS} , asymmetry parameter $\eta = (V_{xx}^{\text{PAS}} - V_{yy}^{\text{PAS}}) / V_{zz}^{\text{PAS}}$ and three Euler angles [1, 7] with the convention $|V_{zz}^{\text{PAS}}| \geq |V_{yy}^{\text{PAS}}| \geq |V_{xx}^{\text{PAS}}|$. As the splitting of nuclear energy levels does not depend on the Euler angles, the occurrence of powder NMR signals is determined by V_{zz}^{PAS} and η only. The superscripts "PAS" can be omitted as long as it will cause no confusion.

3 Slightly Deformed Charge System

Let us consider an assembly of discrete electric charges in PAS. The position change of the N th charge of a small vector $\Delta \mathbf{r} = (\Delta x, \Delta y, \Delta z)$ makes changes of the EFG tensor components (see Fig. 1).

The new charge system is not in PAS and requires re-diagonalization. This fact makes the problem of impact of $\Delta \mathbf{r}$ randomization on V_{zz} and η very complicated, because not only diagonal components of the EFG tensor change but also non-zero off-diagonal elements appear.

The rotations $R(\alpha, \beta, \gamma)$ [11] defined for very small Euler angles may be written as (to the first degree terms in Taylor expansion):

Fig. 1 Position change of the of N th charge of small vector $\Delta \mathbf{r}$

$$\mathbf{R}(\alpha, \beta, \gamma) \approx \begin{bmatrix} 1 & \alpha + \gamma & -\beta \\ -(\alpha + \gamma) & 1 & 0 \\ \beta & 0 & 1 \end{bmatrix},$$

and it transforms any diagonal matrix in the following way:

$$\mathbf{R} \begin{bmatrix} a & 0 & 0 \\ 0 & b & 0 \\ 0 & 0 & c \end{bmatrix} \mathbf{R}^T = \begin{bmatrix} a - b(\alpha + \gamma)^2 + c\beta^2 & (a - b)(\alpha + \gamma) & (c - a)\beta \\ (a - b)(\alpha + \gamma) & b + a(\alpha + \gamma)^2 & -a\beta(\alpha + \gamma) \\ (c - a)\beta & -a\beta(\alpha + \gamma) & c + a\beta^2 \end{bmatrix}$$

$$\approx \begin{bmatrix} a & (a - b)(\alpha + \gamma) & (c - a)\beta \\ (a - b)(\alpha + \gamma) & b & 0 \\ (c - a)\beta & 0 & c \end{bmatrix}.$$

As we can see, to the first degree terms, small rotations do not change the diagonal elements of a matrix; therefore, only the influence of shift of a selected charge on the diagonal components will be taken into account.

In that case, a small shift of N th charge makes a small change of the EFG diagonal components:

$$\Delta V_{ii} \approx \sum_k A_{ik} \Delta x_k,$$

where

$$A_{ik} = \frac{\partial V_{ii}}{\partial x_k^{(N)}}.$$

Further, for convenience, the superscript (N) will be omitted in $x_k^{(N)}$ and $r^{(N)}$ for the N th charge. Then, the explicit form of A_{ik} can be written as

$$A_{ik} = \frac{3x_k}{r^5} \left(1 + 2\delta_{ik} - \frac{5x_i^2}{r^2} \right).$$

We can easily check that $\det A = 0$, which confirms the traceless property of V . No assumption of distribution of variables Δx , Δy , Δz can give the opportunity to obtain a joint distribution of ΔV_{xx} , ΔV_{yy} , ΔV_{zz} . Because, if ΔV_{xx} , ΔV_{yy} are known, ΔV_{zz} can be determined. Therefore, obtaining the distribution of ΔV_{zz} and η parameters may be done through finding a joint distribution of ΔV_{xx} , ΔV_{yy} , which are defined by linear transformation:

$$\begin{bmatrix} \Delta V_{xx} \\ \Delta V_{yy} \end{bmatrix} = \begin{bmatrix} A_{11} & A_{12} & A_{13} \\ A_{21} & A_{22} & A_{23} \end{bmatrix} \begin{bmatrix} \Delta x \\ \Delta y \\ \Delta z \end{bmatrix}. \quad (2)$$

4 Distribution $P_V(V_{xx}, V_{yy})$

The knowledge of P_{xyz} distribution of Δx , Δy , Δz shifts is necessary to obtain the distribution $P_{\Delta V}$ for components ΔV_{xx} , ΔV_{yy} . The assumption that independent but identical Gauss distributions P_s with standard deviation σ_s for each shift is natural due to central limit theorem [12]:

$$P_{xyz}(\Delta x, \Delta y, \Delta z) = \prod_i P_s(\Delta x_i) = \frac{1}{(2\pi)^{3/2} \sigma_s^3} e^{-\frac{\Delta r^2}{2\sigma_s^2}}.$$

Because P_{xyz} is Gaussian and the transformation (2) is linear, $P_{\Delta V}$ is Gaussian too. Thus, we can write directly as follows:

$$\begin{aligned} P_{\Delta V}(\Delta V_{xx}, \Delta V_{yy}) &= \frac{1}{2\pi\sigma_x\sigma_y\sqrt{1-\rho^2}} \exp \\ &\times \left[-\frac{1}{2(1-\rho^2)} \left(\frac{\Delta V_{xx}^2}{\sigma_x^2} + \frac{\Delta V_{yy}^2}{\sigma_y^2} - 2\rho \frac{\Delta V_{xx}\Delta V_{yy}}{\sigma_x\sigma_y} \right) \right]. \end{aligned} \quad (3)$$

We can use this distribution with any three parameters σ_x , σ_y , ρ that are some functions of structural parameters, but their explicit knowledge allows to find dependencies between them and as a result to reduce the number of variables at later numerical modeling. Because the relation (2) maps three to two variables, density transformation can be done using helper coordinate ΔV_h . Then the new distribution $P_{\Delta Vh}(\Delta V_{xx}, \Delta V_{yy}, \Delta V_h)$ can be obtained through the Jacobian, and distribution $P_{\Delta V}$ can be determined by integration out helper coordinate ΔV_h . Let us assume that

$$\Delta V_h = \bar{A} \Delta \mathbf{r}^T, \quad (4)$$

where

$$\bar{\mathbf{A}} = \begin{bmatrix} A_{11} & A_{12} & A_{13} \\ A_{21} & A_{22} & A_{23} \\ 0 & 0 & \frac{6z}{r^5} \end{bmatrix}$$

and

$$\Delta \mathbf{V}_h = \begin{bmatrix} \Delta V_{xx} \\ \Delta V_{yy} \\ \Delta V_h \end{bmatrix}.$$

Then,

$$P_{\Delta V_h}(\Delta \mathbf{V}_h^T) = P_{xyz}(\tilde{\mathbf{A}} \Delta \mathbf{r}^T) \cdot J, \quad (5)$$

where $J = \left| \frac{\partial(\Delta x, \Delta y, \Delta z)}{\partial(\Delta V_{xx}, \Delta V_{yy}, \Delta V_h)} \right|$ is the Jacobian of the transformation (4) and $\tilde{\mathbf{A}} = \bar{\mathbf{A}}^{-1}$. As this transformation is linear, it can be written as follows:

$$J = |\det \tilde{\mathbf{A}}| = \frac{r^{17}}{108xyz(r^2 - 5z^2)},$$

and the matrix $\tilde{\mathbf{A}}$ inversion gives us:

$$\tilde{\mathbf{A}} = \frac{r^5}{6} \begin{bmatrix} -\frac{1}{x} \frac{3r^2 - 5y^2}{r^2 - 5z^2} & \frac{1}{x} \frac{r^2 - 5x^2}{r^2 - 5z^2} & \frac{1}{x} \frac{r^2 - 5x^2}{r^2 - 5z^2} \\ \frac{1}{y} \frac{r^2 - 5y^2}{r^2 - 5z^2} & -\frac{1}{y} \frac{3r^2 - 5x^2}{r^2 - 5z^2} & \frac{1}{y} \frac{r^2 - 5y^2}{r^2 - 5z^2} \\ 0 & 0 & \frac{1}{z} \end{bmatrix}. \quad (6)$$

The direct integration of Eq. (5) allows to join σ_x , σ_y , ρ parameters with $\tilde{A}_{ik}$ components:

$$\begin{aligned} \int P_{\Delta V_h}(\Delta V_{xx}, \Delta V_{yy}, \Delta V_h) d\Delta V_h &= \frac{J}{2\pi C_0 \sigma_s^2} \exp \\ &\times \left[-\frac{C_1^2 \Delta V_{xx}^2 + C_2^2 \Delta V_{yy}^2 - 2C_{12} \Delta V_{xx} \Delta V_{yy}}{2C_0^2 \sigma_s^2} \right], \end{aligned} \quad (7)$$

where

$$\begin{aligned} C_0^2 &= \tilde{A}_{13}^2 + \tilde{A}_{23}^2 + \tilde{A}_{33}^2, \\ C_1^2 &= \tilde{A}_{21}^2 \tilde{A}_{33}^2 + \tilde{A}_{11}^2 \tilde{A}_{33}^2 + \tilde{A}_{11}^2 \tilde{A}_{23}^2 + \tilde{A}_{13}^2 \tilde{A}_{21}^2 - 2\tilde{A}_{11} \tilde{A}_{13} \tilde{A}_{21} \tilde{A}_{23}, \\ C_2^2 &= \tilde{A}_{22}^2 \tilde{A}_{33}^2 + \tilde{A}_{12}^2 \tilde{A}_{33}^2 + \tilde{A}_{12}^2 \tilde{A}_{23}^2 + \tilde{A}_{13}^2 \tilde{A}_{22}^2 - 2\tilde{A}_{12} \tilde{A}_{13} \tilde{A}_{22} \tilde{A}_{23}, \\ C_{12} &= -\tilde{A}_{11} \tilde{A}_{12} \tilde{A}_{23}^2 - \tilde{A}_{21} \tilde{A}_{22} \tilde{A}_{13}^2 - \tilde{A}_{11} \tilde{A}_{12} \tilde{A}_{33}^2 - \tilde{A}_{21} \tilde{A}_{22} \tilde{A}_{33}^2 \\ &\quad + \tilde{A}_{11} \tilde{A}_{13} \tilde{A}_{22} \tilde{A}_{23} + \tilde{A}_{12} \tilde{A}_{13} \tilde{A}_{21} \tilde{A}_{23}. \end{aligned} \quad (8)$$

Comparing (7) with (3) results in:

$$\begin{aligned}\rho &= \frac{C_{12}}{C_1 C_2}, \\ \sigma_x &= \frac{1}{\sqrt{1-\rho^2}} \frac{C_0}{C_1} \sigma_s, \\ \sigma_y &= \frac{1}{\sqrt{1-\rho^2}} \frac{C_0}{C_2} \sigma_s.\end{aligned}\quad (9)$$

Inserting components of matrix (6) to (8) and (9) yields:

$$\begin{aligned}\rho &= \frac{z^4 - y^2 z^2 - x^2 z^2 - 2y^4 + x^2 y^2 - 2x^4}{z^4 + 2x^2 z^2 + 4y^4 + x^4}, \\ \frac{\sigma_x^2}{\sigma_s^2} &= \frac{(x^2 + y^2)(y^2 + z^2)(z^2 + x^2) - x^2 y^2 z^2}{z^4 + 2x^2 z^2 + 4y^4 + x^4} (1 - \rho^2)^{-1}, \\ \sigma_y &= \sigma_x.\end{aligned}\quad (10)$$

The symbolic calculations was partially supported by the Maxima Algebra System.

It is clear that it will not always be possible to determine which specific charge has been shifted, but explicit expressions of distribution parameters (10) allow us to reduce the number of fitting parameters because $\sigma_y = \sigma_x = \sigma$. Thus for diagonal EFG tensor components, taking into account distribution (3), we can write:

$$\begin{aligned}P_V(V_{xx}, V_{yy}) &= \frac{1}{2\pi\sigma^2\sqrt{1-\rho^2}} \exp \left\{ -\frac{1}{2\sigma^2(1-\rho^2)} \right. \\ &\quad \times \left[(V_{xx} - V_{xx}^{(0)})^2 + (V_{yy} - V_{yy}^{(0)})^2 - 2\rho(V_{xx} - V_{xx}^{(0)})(V_{yy} - V_{yy}^{(0)}) \right] \Big\},\end{aligned}\quad (11)$$

where $V_{xx}^{(0)}$ and $V_{yy}^{(0)}$ are the values of unperturbed EFG tensor components.

5 Distribution $p(V_{zz}, \eta)$

Let us notice that V_{zz} and η are parameters that completely define the occurrence of powder NMR signals. Particularly, after the diagonalization of the EFG tensor, V_{zz} is not necessarily the “third” component, and according to the convention $|V_{zz}| \geq |V_{yy}| \geq |V_{xx}|$, EFG tensor requires re-arrangement. Thus, in that case V_{zz} is not a component but positive parameter, while in the previous section V_{xx} and V_{yy} are true EFG tensor components. Dependencies between V_{zz} , η and V_{xx} , V_{yy} are shown in Fig. 2.

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the same way as P_V (through the Jacobian), because f has no unambiguous inverse transformation. Therefore, it is necessary to use a general method of densities transformation [13]:

$$P(V_{zz}, \eta) = \frac{\partial}{\partial V_{zz}} \frac{\partial}{\partial \eta} \int_{f(V_{xx}, V_{yy}) \leq (V_{zz}, \eta)} P_V(V_{xx}, V_{yy}) dV_{xx} dV_{yy}. \quad (12)$$

The scheme of integration areas corresponding to condition $f(V_{xx}, V_{yy}) \leq (V_{zz}, \eta)$ is shown by Fig. 3.

Because direct integration of distribution $P_V(V_{xx}, V_{yy})$ in the form given in (11) over all six areas is very complicated, let us consider some special cases.

5.1 $V_{zz}^{(0)} = 0$

The case where both $V_{xx}^{(0)} = 0$ and $V_{yy}^{(0)} = 0$ corresponds to a regular structure in which there is no electric gradient in the quadrupolar nucleus. The asymmetry parameter is then undetermined. Because quadrupolar interactions are among the strongest in NMR, this situation is defect sensitive. Moreover, because there are no limitations to dispersion σ , the case $V_{zz}^{(0)} = 0$ can be used with isotropic, amorphous solids.

The direct integration of (11) over all six areas gives:

$$\begin{aligned} P(V_{zz}, \eta) = & \frac{V_{zz}}{\pi \sigma^2 \sqrt{1 - \rho^2}} \\ & \times \left\{ \exp \left[-\frac{V_{zz}^2}{4\sigma^2} \frac{1}{1 - \rho^2} (1 + \eta^2 - (1 - \eta^2)\rho) \right] \right. \\ & + \exp \left[-\frac{V_{zz}^2}{2\sigma^2} \frac{1}{1 - \rho^2} \left(\left(\frac{1 - \eta}{2} + \rho \right)^2 + 1 - \rho^2 \right) \right] \\ & \left. + \exp \left[-\frac{V_{zz}^2}{2\sigma^2} \frac{1}{1 - \rho^2} \left(\left(\frac{1 + \eta}{2} + \rho \right)^2 + 1 - \rho^2 \right) \right] \right\}. \end{aligned} \quad (13)$$

Fig. 4 Joint distribution $P(V_{zz}, \eta)$ for $V_{zz}^{(0)} = 0$, $\rho = 0$ and $\sigma = 1$

The joint distribution (13) of V_{zz} and η in this case is presented in Fig. 4.

5.2 $V_{zz}^{(0)} \gg 0$

When $V_{zz}^{(0)} \gg 0$, then the density (11) can be integrated only over areas in which the distribution is substantially different from 0. For η significantly different from 1, the integration can be done over area I only. Using transformation (12), the direct integration of (11) gives:

$$\begin{aligned}
 P(V_{zz}, \eta) \approx & \frac{V_{zz}}{4\pi\sigma^2\sqrt{1-\rho^2}} \\
 & \times \left\{ \exp \left[-\frac{1}{4\sigma^2} \left(\frac{(V_{zz}\eta - V_{zz}^{(0)}\eta^{(0)})^2}{1-\rho} + \frac{(V_{zz} - V_{zz}^{(0)})^2}{1+\rho} \right) \right] \right. \\
 & \left. + \exp \left[-\frac{1}{4\sigma^2} \left(\frac{(V_{zz}\eta + V_{zz}^{(0)}\eta^{(0)})^2}{1-\rho} + \frac{(V_{zz} - V_{zz}^{(0)})^2}{1+\rho} \right) \right] \right\}. \quad (14)
 \end{aligned}$$

When η is close to 1, an integration over area II should be added. In this case, the $P_{add}(V_{zz}, \eta)$ addition should be applied to the formula (14):

$$\begin{aligned}
 P_{add}(V_{zz}, \eta) = & \frac{V_{zz}}{4\pi\sigma^2\sqrt{1-\rho^2}} \\
 & \times \left\{ \exp \left[-\frac{1}{2\sigma^2(1-\rho^2)} \left(\left(V_{zz} - V_{zz}^{(0)} \frac{1+\eta^{(0)}}{2} \right)^2 \right. \right. \\
 & \quad \left. \left. + \left(V_{zz} \frac{1-\eta}{2} - V_{zz}^{(0)} \frac{1-\eta^{(0)}}{2} \right)^2 \right. \right. \\
 & \quad \left. \left. - 2\rho \left(V_{zz} - V_{zz}^{(0)} \frac{1+\eta^{(0)}}{2} \right) \left(V_{zz} \frac{1-\eta}{2} - V_{zz}^{(0)} \frac{1-\eta^{(0)}}{2} \right) \right) \right] \right. \\
 & \left. + \exp \left[-\frac{1}{2\sigma^2(1-\rho^2)} \left(\left(V_{zz} - V_{zz}^{(0)} \frac{1+\eta^{(0)}}{2} \right)^2 \right. \right. \right. \\
 & \quad \left. \left. + \left(V_{zz} \frac{1+\eta}{2} - V_{zz}^{(0)} \frac{1-\eta^{(0)}}{2} \right)^2 \right. \right. \\
 & \quad \left. \left. - 2\rho \left(V_{zz} - V_{zz}^{(0)} \frac{1+\eta^{(0)}}{2} \right) \left(V_{zz} \frac{1+\eta}{2} - V_{zz}^{(0)} \frac{1-\eta^{(0)}}{2} \right) \right) \right] \right\}. \quad (15)
 \end{aligned}$$

Fig. 5 Joint distribution $P(V_{zz}, \eta)$ for $V_{zz}^{(0)} = 1, \rho = 0$, $\sigma = 0.15$ and **a** $\eta^{(0)} = 0$, **b** $\eta^{(0)} = 0.5$, **c** $\eta^{(0)} = 1$

It should be noted that the formula (14) even with the above correction (15) is only approximate and it does not normalize to 1. The sum of joint distributions (14) and (15) is shown in Fig. 5.

Fig. 6 Central transition MAS NMR spectra of quadrupolar nuclei for $\eta^{(0)} = 0$, $V_{zz}^{(0)} = \text{const}$ and: **a** $\sigma = 0$, $\rho = 0$, **b** $\sigma = 0.08V_{zz}$, $\rho = 0$, **c** $\sigma = 0.16V_{zz}$, $\rho = 0$, **d** $\sigma = 0.08V_{zz}$, $\rho = 0.95$

6 NMR Spectra

The influence of dispersion of V_{zz} and η on NMR signals is shown by the example spectra in Fig. 6 for several dispersion parameters.

These spectra were obtained according to the theory presented in [1] for central transition (CT) NMR of quadrupolar nuclei in the magic angle spinning (MAS) regime by taking into account the dispersion (14) calculated in this work.

7 Summary

The joint dispersion of electric field gradient tensor components was made directly from the disturbance of the initial electric charge system surrounding the quadrupolar nucleus. In addition to that, the dependence between the structural and the obtained dispersion parameters was calculated, which resulted in the reduction of the number of dispersion parameters. The theory presented in this work can be useful, owing to the analytic form of the obtained distributions, for the modeling of NMR signals in disordered compounds with quadrupolar interactions where parameters are scattered around initial magnitudes. The influence

of the obtained theory on NMR signals has been presented in this work with the example central transition MAS NMR spectra for several cases.

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