Multiple quantum NMR in solids as a method of determination of Wigner–Yanase skew information

S. I. Doronin\textsuperscript{a}, E. B. Fel’dman\textsuperscript{a}, I. D. Lazarev\textsuperscript{a,b}

\textsuperscript{a}Institute of Problems of Chemical Physics of Russian Academy of Sciences, Chernogolovka, Moscow Region, Russia 142432
\textsuperscript{b}Faculty of Fundamental Physical-Chemical Engineering, Lomonosov Moscow State University, GSP-1, Moscow, Russia 119991

Abstract

A connection of the Wigner–Yanase skew information and multiple quantum (MQ) NMR coherences is considered at different temperatures and evolution times of nuclear spins with dipole-dipole interactions in MQ NMR experiments in solids. It is shown that the Wigner–Yanase skew information at temperature $T$ is equal to the double second moment of the MQ NMR spectrum at the double temperature for any evolution times. A comparison of the many-spin entanglement obtained with the Wigner–Yanase information and the Fisher information is conducted.

Keywords: many-spin entanglement, Fisher information, Wigner-Yanase skew information, multiple quantum NMR, multiple quantum coherences, second moment, temperature

1. Introduction

The Wigner–Yanase skew information \cite{1, 2, 3, 4} together with the Fisher information \cite{5, 6} allow the development of powerful methods for the investigation of entanglement, including many–particle entanglement \cite{7, 8}. Further investigations of many–particle entanglement require the development of corresponding experimental methods. In particular, it was shown \cite{7, 9} that a lower bound on the quantum Fisher information \cite{5, 6} coincides with the double second moment of the spectrum of multiple quantum (MQ) coherences. As a result, the lower bound on the quantum Fisher information can be found in MQ NMR experiments \cite{10}, in cold–atom experiments, including experiments with Bose–Einstein condensates, ultracold atoms in cavities, and
trapped ions [11, 12, 13, 14, 15]. Using the properties of the quantum Fisher information one can obtain the number of the entangled particles (spins) in the system under consideration [7] and even find the dependence of the number of the entangled spins on the temperature [9].

The Wigner–Yanase skew information [1, 2, 3, 4] is also connected with the spectrum of MQ coherences. In particular, we demonstrate in the present article that the Wigner–Yanase skew information in a spin system \( s = 1/2 \) at the system temperature \( T \) equals the double second moment of the MQ NMR spectrum obtained at the temperature \( 2T \). Using the properties of the Wigner–Yanase skew information one can investigate many–spin entanglement on the basis of the MQ NMR spectroscopy [10].

The main aim of the present article is the development of a method of extracting the Wigner–Yanase skew information from the MQ NMR spectra. We also compare on the simple models [8, 16] the many–spin entanglement obtained both with the Wigner–Yanase information and the Fisher information.

The article is organized as follows. In Sec. 2 a short introduction to the MQ NMR spectroscopy is given. The connection of the Wigner–Yanase skew information with the second moment of the MQ NMR spectrum is obtained in Sec. 3. A comparison of many–spin entanglement obtained with the Wigner–Yanase and the Fisher information on simple models [8, 16] is conducted in Sec. 4. We briefly discuss our results in concluding Sec. 5.

2. MQ NMR for solving problems of quantum informatics

MQ NMR methods are widely used for solving problems of quantum informatics [17, 18]. The MQ NMR experiment consists of four distinct periods of time as depicted in Fig. 1: preparation (\( \tau \)), evolution (\( t_1 \)), mixing (\( \tau \)), and detection (\( t_2 \)) [10]. MQ NMR coherences are created by a periodic multipulse sequence, consisting of \( \pm x \)-pulses, irradiating the system of the preparation period [10]. If the inverse period of the multipulse sequence significantly exceeds the local dipolar field (in frequency units) [19] then MQ NMR dynamics can be described by the averaged nonsecular two–spin/two–quantum Hamiltonian \( H_{MQ} \) [20]

\[
H_{MQ} = H^{(+2)} + H^{(-2)}, \quad H^{(\pm 2)} = \frac{1}{2} \sum_{j<k} D_{jk} I_j^\pm I_k^\pm, \quad (1)
\]
where $D_{jk}$ is the coupling constant between spins $j$ and $k$, and $I^+_j, I^-_j$ are the raising and lowering operators of spin $j$. On the mixing period, the spin system is irradiated by the multiple pulse sequence with $\pm y$-pulses. As a result, the averaged nonsecular two-spin/two quantum Hamiltonian on the mixing period equals $(-H_{MQ})$ [10].

In order to investigate the MQ NMR dynamics of the system on the preparation period [10] one should find the density matrix $\rho(t)$ by solving the Liouville evolution equation [19]

$$i \frac{d\rho(t)}{dt} = [H_{MQ}, \rho(t)]$$

with the initial thermodynamic equilibrium density matrix

$$\rho(0) = \rho_{eq} = \frac{\exp(\frac{\hbar \omega_0}{kT} I_z)}{Z},$$

where $Z = Tr \{ \exp(\frac{\hbar \omega_0}{kT} I_z) \}$ is the partition function, $\hbar$ and $k$ are the Plank and Boltzmann constants, respectively, $\omega_0$ is the Larmor frequency, $T$ is the temperature, and $I_z$ is the operator of the projection of the total spin angular momentum on the z-axis, which is directed along the strong external magnetic field.

Following the preparation, evolution, and mixing periods of the MQ NMR experiments and taking into account the phase increment $\phi$ of the radio-frequency pulses [10], the resulting signal $G(\tau, \phi)$ stored as population infor-
The signal $G(\tau, \phi)$ of the MQ NMR [10] can be rewritten as

$$G(\tau, \phi) = \sum_n e^{in\phi} \text{Tr} \{ \rho_{\text{pre}, n}(\tau, \beta) \rho_{\text{pre}, -n}(\tau, \beta) \},$$

where we took into account that

$$[I_z, \rho_{\text{pre}, n}] = n \rho_{\text{pre}, n}$$

The normalized intensities of the MQ NMR coherences can be determined as follows

$$J_n(\tau, \beta) = \frac{T \{ \rho_{\text{pre}, n}(\tau, \beta) \rho_{\text{pre}, -n}(\tau, \beta) \}}{\text{Tr}(\rho_{\text{eq}}^2)}$$

As was shown in [8],

$$\text{Tr}(\rho_{\text{eq}}^2) = \frac{2^N c h^N(\beta)}{Z^2},$$

where $N$ is the number of the spins. It was also shown that

$$\sum_n J_n(\tau, \beta) = 1$$

The second moment (dispersion) $M_2(\tau, \beta)$ of the distribution of the MQ NMR coherences $J_n(\tau, \beta)$ can be calculated from Eq. [7] according to [22]

$$M_2(\tau, \beta) = -\frac{1}{G(\tau, \beta)} \left. \frac{d^2 G(\tau + t, \beta)}{dt^2} \right|_{t=0}$$
Using Eqs. (7,8,12) one can obtain

\[ M_2(\tau, \beta) = \sum_n n^2 J_n(\tau, \beta) \]  
(13)

A lower bound on the quantum Fisher information coincides with the double second moment of Eq. (13) [7, 9]. As a result, the analysis of the temperature dependence of the second moment \( M_2(\tau, \beta) \) of the distribution of the intensities of the MQ NMR coherences allows us to obtain the number of the entangled spins at different temperatures [8]. In the following Sec. 3 we demonstrate that the Wigner–Yanase skew information is also connected with the second moment \( M_2(\tau, \beta) \) and can be useful for the investigation of many-spin entanglement.

3. The Wigner–Yanase skew information and MQ NMR

The Wigner–Yanase skew information is defined as [1, 2, 3, 4]

\[ I_{\text{WY}}(\rho(\tau, \beta), I_z) = -\frac{1}{2} \text{Tr}([\sqrt{\rho(\tau, \beta)}, I_z]^2) = -2\text{Tr}([\sqrt{\rho(\tau, \beta)}, I_z])^2, \]  
(14)

where the Pauli operator \( \sigma_z = 2I_z \). Introducing the evolution operator

\[ V(\tau) = e^{iH_{\text{MQ}}\tau} \]  
(15)

and using Eq. (3) one can write the density matrix \( \rho(\tau, \beta) \) as follows:

\[ \rho(\tau, \beta) = V^+(\tau) \frac{e^{\beta I_z}}{Z} V(\tau) \]  
(16)

Now we use the evident relationship:

\[ \sqrt{\rho(\tau, \beta)} = \frac{1}{V^+(\tau)} \frac{e^{\beta I_z}}{Z} V(\tau) = \frac{e^{\beta I_z}}{\sqrt{Z}} V(\tau). \]  
(17)

It can be proved by simple calculation:

\[ \sqrt{\rho} \sqrt{\rho} = V^+(\tau) \frac{e^{2\beta I_z}}{\sqrt{Z}} V(\tau) V^+(\tau) \frac{e^{2\beta I_z}}{\sqrt{Z}} V(\tau) = V^+(\tau) \frac{e^{2\beta I_z}}{Z} V(\tau) = \rho(\tau, \beta) \]  
(18)

Then we have

\[ [I_z, \sqrt{\rho(\tau, \beta)}] = \left[ I_z, \sum_k \rho_k \left( \tau, \frac{\beta}{2} \right) \right] = \sum_k k \rho_k \left( \tau, \frac{\beta}{2} \right), \]  
(19)
Finally, one can obtain that

\[
I_{WY}(\rho(\tau, \beta), I_z) = 2 \sum_k k^2 J_k \left(\tau, \frac{\beta}{2}\right) = 2M_2 \left(\tau, \frac{\beta}{2}\right)
\]

Thus, we obtain an important observation. If the spin system is investigated with MQ NMR at the temperature \( T \sim \beta^{-1} \) then the Wigner–Yanase skew information equals to the double second moment of the distribution of the intensities of the MQ NMR coherences at the temperature \( 2T \sim 2\beta^{-1} \) at any time during the spin evolution.

The Wigner-Yanase skew information is connected with the second moment of the distribution of the MQ NMR coherences analogously to the Fisher information. We compare these informations in the following Section 4.

4. The comparison of the many-spin entanglement obtained with the Wigner–Yanase information and the Fisher information

The Wigner–Yanase skew information \( I_{WY}(\rho(\tau, \beta), I_z) \) and the Fisher information \( I_F(\rho(\tau, \beta), I_z) \) can be used for the investigation of the many-spin entanglement. Indeed, it is known [5, 6] that if \( I_{WY}(\rho(\tau, \beta), I_z) \) or \( I_F(\rho(\tau, \beta), I_z) \) exceeds \( mk^2 + (N - mk)^2 \), where \( k, m \) are integer and \( m \) is the integer part of \( N/k \), then we have \( N_{\text{ent}} = (k+1) \) - particle entangled spins in the system. The informations are connected by the following restriction [3]

\[
I_{WY}(\rho(\tau, \beta), I_z) \leq I_F(\rho(\tau, \beta), I_z) \leq 2I_{WY}(\rho(\tau, \beta), I_z).
\]

The restrictions (22) allow us to hope that the obtained results for the number of the entangled spins are not very different. For the comparison we used the model [23] of a nonspherical nanopore filled with a gas of spin-carrying atoms (for example, xenon) or molecules in a strong external magnetic field. This model allows the investigation of the many-spin entanglement in the spin system consisting of hundreds of nuclear spins [8].

We investigated many-spin entanglement in the spin system, consisting of 201 spins, in a nanopore both with the Wigner–Yanase information and the Fisher information.
Figure 2: The dependence of the number of the entangled spins on the inverse temperature $\beta = \frac{\pi \omega}{kT}$; black circles - the results are obtained with the Fisher information; open circles - the results are obtained with the Wigner–Yanase information.
Figure 3: The dependence of the number $N_{\text{ent}}$ of the entangled spins on the parameter $\beta$ (the inverse temperature) for zigzag chains consisting of six spins.
$I_{WY}(\rho(\tau, \beta), I_z)$ and the Fisher information $I_F(\rho(\tau, \beta), I_z)$. In Fig. 2 the dependence of the number of the entangled spins on the inverse temperature is presented. Fig. 2 demonstrates that the number of the entangled spins increases when the temperature decreases both for the Wigner–Yanase information and the Fisher information.

An analogous investigation was conducted on the model of the proton zigzag chain in a single crystal of hambergite [16, 24]. In Fig. 3, similar results on many-spin entanglement are presented for the system consisting of six spins at different temperatures for both used informations.

5. Conclusion

We studied the connection of the Wigner–Yanase skew information with the second moment of the distribution of the intensities of MQ coherences in the MQ NMR experiment. It was shown that the Wigner–Yanase skew information at the temperature $T \sim \beta^{-1}$ equals the double second momentum of the MQ NMR spectrum at the temperature $2T \sim 2\beta^{-1}$. We compare also the results on the many-spin entanglement obtained with the Wigner–Yanase skew information and the Fisher information.

6. Acknowledgement

We acknowledge funding from the Ministry of Science and Higher Education of the Russian Federation (Grant No. 075-15-2020-779).

References

[1] E.P.Wigner, M.M. Yanase, Proc.Nat.Acad.Sei. USA 49, 910-918 (1963)
[2] S.Luo, Phys.Rev.Lett. 91, 180403 (2003)
[3] S.Luo, Proc.Amer. Math.Soc. 132, No.885-890 (2003)
[4] Z.Chen, Phys.Rev. A 71, 052302 (2005)
[5] G.Toth, I.Apellaniz, J. Phys. A 47, 424006 (2014)
[6] L.Pezze, A.Smerzi, M.K. Oberthaler, R. Schmied, P.Treutlein, Rev.Mod.Phys. 90, 035005 (2018)
[7] M.Gartner, P.Hauke, A.M.Rey, Phys.Rev.Lett. 120, 040402 (2018)
[8] S.I.Doronin, E.B.Fel’dman, I.D.Lazarev, Phys. Rev. A 100,022330 (2019)
[9] D.Girolami, B.Yadin,Entropy 19,124 (2017)
[10] J.Baum, M.Munowitz, A.N.Garroway, A.Pines, J.Chem.Phys. 83, 2015 (1985)
[11] B. Swingle, G. Bentsen, M. Scheleier-Smith, P. Hayden, Phys. Rev. A 94, 040302 (2010)
[12] F.M. Cucchietti, J.Opt.Soc. Am. B27, A30 (2010)
[13] I.D. Leroux, M.H. Schleier-Smith, V.Vuletic, Phys.Rev.Lett. 104, 073602 (2010)
[14] T.Macri, A. Smerzi, L.Pezze, Phys.Rev. A 94, 010102 (2016)
[15] M.Gartner, J.G.Bohnet, A.Safavi-Naini, M.L. Wall, J.J. Bollinger, A.M.Rey, Nat.Phys. 13, 781 (2017)
[16] G.A.Bochkin, S.G.Vasil’ev, S.I. Doronin, E.I.Kuznetsova, I.D.Lazarev, E.B.Fel’dman, Appl.Magn.Reson. 51, 667-678 (2020)
[17] E.B.Fel’dman, A.N. Pyrkov, A.I.Zenchuk, Philos. Trans. R. Soc. London A 370, 4690 (2012)
[18] G.B.Furman, V.M.Meerovich, V.L.Sokolovsky, Phys. Rev. A 78 042301 (2008)
[19] M.Goldman. Spin temperature and nuclear magnetic resonance in solids, Oxford,UK, Clarendon Press. 1970.
[20] S.I.Doronin, I.I.Maksimov, E.B.Fel’dman, J. Exp. Theor. Phys. 91, 597 (2000)
[21] E.B.Fel’dman, S.Lacelle, Chem.Phys.Lett. 253, 27 (1996)
[22] A.Abragam, The Principles of Nuclear Magnetism, Clarendon. Oxford. 1961
[23] J. Baugh, A. Kleinhammes, D. Han, Q. Wang, Y. Wu, Science 294, 1505 (2001)

[24] G.A. Bochkin, E.B. Fel’dman, E.B. Kuznetsova, I.D. Lasarev, S.G. Vasil’ev, V.I. Volkov, J. Magn. Reson. 319, 106816 (2020)