Cumhuriyet Sci. J., 43(3) (2022) 510-514
DOI: https://doi.org/10.17776/csj.1083228

Cumhuriyet Science Journal

| csj.cumhuriyet.edu.tr | Founded: 2002 ISSN: 2587-2680 e-ISSN: 2587-246X Publisher: Sivas Cumhuriyet University

Rx, Ry and Rz Rotation Operators of Spin 4 Systems in Quantum Information Theory

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Research Article

History
Received: 05/03/2022
Accepted: 01/07/2022

ABSTRACT

Quantum computing requires use of various physical techniques together with quantum theory. One of the promising systems is spin systems as applied and seen in pulsed nuclear magnetic resonance (NMR) and pulsed electron paramagnetic resonance (EPR) spectroscopies and hence spin-based quantum information technology. Construction of higher spin systems and related rotation operators is important for the theoretical infrastructure that can be used in quantum information theory. It is expected that as the value of spin increases, it will give way to longer time in the computation with bigger data.

Spin operators up to spin-4 have been published in previous studies. In this work, explicit symbolic expressions of x, y and z components of rotation operators for spin-4 were worked out via exponential operator for each element of related spin operator matrices and simple linear curve fitting process. The procedures gave out exact expressions of each element of the rotation operators. It can be predicted that quantum rotation operators for higher spins, like spin-4, will theoretically and practically contribute to spin-based quantum information technology.

Keywords: Rotation operator, Spin, Quantum computers, Quantum information theory, Linear curve fitting process.

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Introduction

Quantum computing combines computer science with quantum mechanics and it is a fast-growing research field[1-5]. Feynman [6,7] pointed out that only the computers working with quantum mechanical principles can simulate a quantum mechanical system, or one needs a quantum computer utilizing quantum mechanical processes can succeed such sophisticated and time-consuming works. One system of such computers utilizes spins and hence spin rotation operators, also known as completely quantum mechanical rotation operators and have no classical counterpart.

Spin rotation operators are one of the processes in quantum mechanical applications like pulsed magnetic resonance spectroscopy. In the literature only rotation operators of spin-1/2 system R̂_x (θ),R̂_y (θ),R̂_z (θ) can be found related with quantum information theory. Wigner[8] introduced expressions of rotation matrices or Wigner–d matrices for orbital angular momenta on the standard Euler angles basis. Real rotation operators for total angular momenta of spin-1/2, 1, 3/2 and 2 were generated from Wigner–d formula in some quantum mechanics textbooks[9-12] and in some published papers [13-19]. A recently published paper on rotation operators by Curtright et al. [20] and Curtright and Van Kortryk[21] give rotation operator expressions in polynomial form for all spins in Cartesian components. In order to find out the rotation operators in a matrix form one has to sum up the polynomial terms given, which includes powers of related angular momentum operators.

Pulsed nuclear magnetic resonance (pulsed-NMR), pulsed electron paramagnetic resonance (pulsed-EPR) and pulsed electron nuclear double resonance (pulsed-ENDOR) spectroscopies, however, utilize rotation operators in rotating coordinate system or laboratory coordinate system where the spins are polarized along a definite orientation by an external magnetic field. The direction of the external magnetic field is defined as z–axis and a series of magnetic pulses are applied consequently along laboratory x and/or y axes to rotate the polarized spins around related axes. Spin-based quantum-computation systems, where pulsed magnetic resonances are leading techniques which utilize pulse sequences, use the rotation operators intensively in the rotating coordinate system[22-28].

Electron spin has attracted renewed interest towards the development of various new devices that depend on combined logic, storage and sensor applications. Another important application of these spin-based devices is in the computation depending on the quantum logic. Spin-based quantum computation depending on electronic solid-state devices are shifting gradually toward the prospective information technology [28].

In this work, explicit rotation operator expressions of spin-4 are constructed from exponential operators given in Eqn. (1) for x, y and z components of angular momenta for a series of angles θ between interval θ_1 and θ_N with certain steps, e.g between 0 and 360o with 10o steps, and fitting the obtained values to suitable functions by linear curve fitting procedure.

Obtaining Rotation Processors

Matrix representations of rotation operators and their effect on quantum states are essential part of the quantum mechanics of microscopic systems [3-8] and these matrices, in turn, can be widely used in a variety of applications. In order to be able to perform processes with exponential rotation operators given in Eqn. (1), it is necessary to form this operator for processing as linear operator, in other words, this operator should be linearized by making series expansions given as

$$\hat{R}_\alpha = \exp\left(i\theta_p \hat{J}_\alpha\right), \quad \alpha = x, y, z \tag{1}$$

which is derived from time dependent Schrödinger equation $-i\hbar\frac{\partial\psi}{\partial t} = \widehat{\mathcal{H}}\psi$ for a rotating magnetic field pulse B_1, where $\widehat{\mathcal{H}} = g\beta B_1 \hat{J}_\alpha$ is pulse Hamiltonian applied to a spin system polarized by an external magnetic field along laboratory *x* or *y* axis and $\hat{J}_\alpha$ $(\alpha = x, y, z)$ are Pauli spin matrices representing electron spin *S* or nuclear spin *I*, coupled *S* and *I* systems. The constants g and β are Landé-g factor and Bohr magneton respectively. Here θ_p is the angle of rotation and t_p is rotating pulse duration. Thus θ_p can be written as $\theta_p = g\beta B_1 t_p/\hbar = \omega_p t_p$.

Eqn. (1) can be rewritten by definition

$$\mathrm{R}_\alpha = \exp\left(\mathrm{i}\theta_\mathrm{p}\hat{J}_\alpha\right) = \cos\left(\theta_\mathrm{p}\hat{J}_\alpha\right) + i\sin\left(\theta_\mathrm{p}\hat{J}_\alpha\right), \quad \alpha = \mathrm{x,y,z} \tag{2}$$

Where

$$\cos\left(\theta_p\hat{J}_\alpha\right) = \mathbb{I} - \frac{1}{2!}\theta_p^2\hat{J}_\alpha^2 + \frac{1}{4!}\theta_p^4\hat{J}_\alpha^4 - \frac{1}{6!}\theta_p^6\hat{J}_\alpha^6 + \cdots = \sum_{n=0}^{\infty}\frac{1}{(2n)!}\theta_p^{2n}\hat{J}_\alpha^{2n} \tag{3}$$

$$\sin\left(\theta_p\hat{J}_\alpha\right) = \frac{1}{1!}\theta_p^1\hat{J}_\alpha^1 - \frac{1}{3!}\theta_p^3\hat{J}_\alpha^3 + \frac{1}{5!}\theta_p^5\hat{J}_\alpha^5 - \cdots = \sum_{n=0}^{\infty}\frac{1}{(2n+1)!}\theta_p^{2n+1}\hat{J}_\alpha^{2n+1}$$

As the spin value increases evaluation of power series given in Eqn. (3) requires intensive calculation due to the powers of spin operator matrices. Pauli matrices for spin-1/2 and corresponding explicit rotation operators are borrowed from textbooks [11-13] and are given in Eqn. (4).

$$\hat{I}_x = \frac{1}{2}\begin{bmatrix}0 & 1\\1 & 0\end{bmatrix}, \hat{I}_y = \frac{i}{2}\begin{bmatrix}0 & -1\\1 & 0\end{bmatrix}, \hat{I}_z = \frac{1}{2}\begin{bmatrix}1 & 0\\0 & -1\end{bmatrix} \tag{4}$$

$$\hat{R}_x(\theta) = \begin{bmatrix}c & is\\is & c\end{bmatrix}, \hat{R}_y(\theta) = \begin{bmatrix}c & s\\-s & c\end{bmatrix}, \hat{R}_z(\theta) = \begin{bmatrix}z & 0\\0 & z^*\end{bmatrix}$$

where c, s and z are defined as $c = \cos(\theta/2)$, $s = \sin(\theta/2)$, $z = c + is$. The rotation operators for spin-1/2 systems are rather easy because the elements of the powers of Pauli spin matrices are either zero or unity multiplied by a coefficient.

One of the way of obtaining explicit expressions of the rotation operators for the spins greater than 1/2 can be done two-step numerical calculation. In the first step the sine and cosine series given in Eqn. (3) are summed up numerically to highest possible precision for each element of a spin matrix for certain angles between e.g. 0° and 360° with definite intervals like 10°. Variations of real and imaginary elements of rotation matrices are numerical values obtained after sums obtained for each angle. In the second step, variations of each element of the rotation matrices as functions of rotation angles are fitted to a linear function. The exact fitting function $r_{ij}(\theta)$, found after some trials, are determined and given in Eqn. (5),

$$r_{ij}(\theta) = \sum_{p=1}^{K}\xi_p^{(ij)}\cos^{K-p}\left(\frac{\theta}{2}\right)\sin^{p-1}\left(\frac{\theta}{2}\right) \tag{5}$$

where $K = 2(J+1)$; $i, j = 1, 2, 3 \cdots K$, θ is rotation angle around *x, y* or *z* axis and J is the value of spin (nuclear, electronic or coupled spins) and K is the number of terms of fitting function and ξ_p is the coefficient of *p*'th term of linear fitting function which is determined by linear curve fitting process. The accuracies of all fitting processes were controlled by the value *r* which is known as goodness of fitting, and visually on simultaneous plots of original and fitted curves. The operators corresponding to spins smaller than 4 were published previously [29-30]. All rotation operator matrices obtained were tested by comparing to corresponding operators obtained from Wigner–d formula [8,19] and operators in polynomial equations given by Curtright *et al*. [20] and Curtright and Van Kortryk [21].

Results and Discussion

Rotation operator elements corresponding to spin-4 operators are calculated using Eqns. (3) and (5), as discusses in the text above. The compact fit function given in Eqn. (5) can be expanded as given below,

$$r_{ij} = \xi_0 c^8 + \xi_1 c^7 s^1 + \xi_2 c^6 s^2 + \xi_3 c^5 s^3 + \xi_4 c^4 s^4 + \xi_5 c^3 s^5 + \xi_6 c^2 s^6 + \xi_7 c^1 s^7 + \xi_8 s^8 \tag{6}$$

Angular variation of rotation operator element r_{26} of operator matrix $R_x(\theta)$ and as an example, is given in Figure 1a. Angular variation of rotation operator element r_{46} of operator matrix $R_y(\theta)$, as an example, is given in Figure 1b.

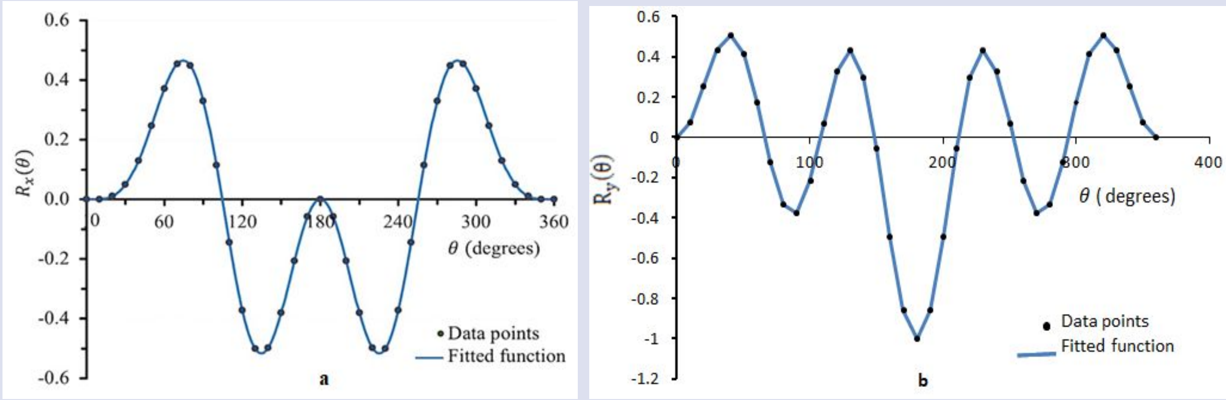

Figure 1. a) The variation of the element r_{26} of the rotation operator $R_x(\theta)$ for spin-4 with rotation angle. b) The variation of the element r_{46} of the rotation operator $R_y(\theta)$ for spin-4 with rotation angle.

The variation and graph of these elements according to the angle are given in Figure 1 a and b. As can be seen in Figure 1, the agreement was found to be perfect in the operations performed with the least squares method. Figure 1 shows the solid line fit function in a and b.

$$r_{26} = \sqrt{175}\, c^4 s^4 - \sqrt{63}\, c^2 s^6 \qquad (7)$$

$$R_x = \begin{bmatrix} r_{11} & ir_{12} & r_{13} & ir_{14} & r_{15} & ir_{16} & r_{17} & ir_{18} & r_{19} \\ ir_{12} & r_{22} & ir_{23} & r_{24} & ir_{25} & r_{26} & ir_{27} & r_{28} & ir_{18} \\ r_{13} & ir_{23} & r_{33} & ir_{34} & r_{35} & ir_{36} & r_{37} & ir_{27} & r_{17} \\ ir_{14} & r_{24} & ir_{34} & r_{44} & ir_{45} & r_{46} & ir_{36} & r_{26} & ir_{16} \\ r_{15} & ir_{25} & r_{35} & ir_{45} & r_{55} & ir_{45} & r_{35} & ir_{25} & r_{15} \\ ir_{16} & r_{26} & ir_{36} & r_{46} & ir_{45} & r_{44} & ir_{34} & r_{24} & ir_{14} \\ r_{17} & ir_{27} & r_{37} & ir_{36} & r_{35} & ir_{34} & r_{33} & ir_{23} & r_{13} \\ ir_{18} & r_{28} & ir_{27} & r_{26} & ir_{25} & r_{24} & ir_{23} & r_{22} & ir_{12} \\ r_{19} & ir_{18} & r_{17} & ir_{16} & r_{15} & ir_{14} & r_{13} & ir_{12} & r_{11} \end{bmatrix}$$

$$R_y = \begin{bmatrix} r_{11} & r_{12} & -r_{13} & -r_{14} & r_{15} & r_{16} & -r_{17} & -r_{18} & r_{19} \\ -r_{12} & r_{22} & r_{23} & -r_{24} & -r_{25} & r_{26} & r_{27} & -r_{28} & -r_{18} \\ -r_{13} & -r_{23} & r_{33} & r_{34} & -r_{35} & r_{36} & r_{37} & r_{27} & -r_{17} \\ r_{14} & -r_{24} & -r_{34} & r_{44} & r_{45} & -r_{46} & r_{36} & r_{26} & r_{16} \\ r_{15} & r_{25} & -r_{35} & -r_{45} & r_{55} & r_{45} & -r_{35} & -r_{25} & r_{15} \\ -r_{16} & r_{26} & -r_{36} & -r_{46} & -r_{45} & r_{44} & r_{34} & -r_{24} & -r_{14} \\ -r_{17} & -r_{27} & r_{37} & -r_{36} & -r_{35} & -r_{34} & r_{33} & r_{23} & -r_{13} \\ r_{18} & -r_{28} & -r_{27} & r_{26} & r_{25} & -r_{24} & -r_{23} & r_{22} & r_{12} \\ r_{19} & r_{18} & -r_{17} & -r_{16} & r_{15} & r_{14} & -r_{13} & -r_{12} & r_{11} \end{bmatrix}$$

$$R_z = \begin{bmatrix} z_{11} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & z_{22} & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & z_{33} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & z_{44} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & z_{55} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & {z_{44}}^* & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & {z_{33}}^* & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & {z_{22}}^* & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & {z_{11}}^* \end{bmatrix}$$

where other coefficients are zero. All nonzero elements of rotation operator matrices $R_x(\theta)$, $R_y(\theta)$ and $R_z(\theta)$ were calculated similarly. Calculations were performed with the precision of $\varepsilon = 10^{-9}$ and elements of rotation operators were given in Eqn. (8) and Table1.

Table 1. Elements of rotation operators for spin 4

$r_{11} = c^8$	$r_{28} = s^8 - \sqrt{49}c^2s^6$
$r_{12} = \sqrt{7}c^7$	$r_{33} = c^8 - \sqrt{144}c^6s^2$
$r_{13} = -\sqrt{28}\,c^6s^2$	$r_{34} = \sqrt{18}c^7s - \sqrt{450}c^5s^3 + \sqrt{200}c^3s^5$
$r_{14} = -\sqrt{56}c^5s^3$	$r_{35} = \sqrt{640}c^4s^4 - \sqrt{90}(c^6s^2 + c^2s^6)$
$r_{15} = \sqrt{70}c^4s^4$	$r_{36} = \sqrt{200}c^5s^3 + \sqrt{450}c^3s^5 - \sqrt{18}cs^7$
$r_{16} = \sqrt{56}c^3s^5$	$r_{37} = \sqrt{225}c^4s^4 - \sqrt{144}c^2s^6 + s^8$
$r_{17} = -\sqrt{28}c^2s^6$	$r_{44} = c^8 - \sqrt{225}c^6s^2 + \sqrt{900}c^4s^4 - \sqrt{100}c^2s^6$
$r_{18} = -\sqrt{7}cs^7$	$r_{45} = \sqrt{20}(c^7s + cs^7) + \sqrt{720}(c^3s^5 - c^5s^3)$
$r_{19} = s^8$	$r_{46} = s^8 - \sqrt{100}c^6s^2 + \sqrt{900}c^4s^4 - \sqrt{225}c^2s^6$
$r_{22} = c^8 - \sqrt{49}c^6s^2$	$r_{55} = c^8 - \sqrt{256}(c^6s^2 + c^2s^6) + s^8$
$r_{23} = \sqrt{14}c^7s - \sqrt{126}c^5s^3$	$z_{11} = c^8 - 28(c^6s^2 + c^2s^6) + 70c^4s^4 + s^8 + 8i(c^7s - cs^7) + 56i(c^3s^5 - c^5s^3)$
$r_{24} = \sqrt{175}c^4s^4 - \sqrt{63}c^6s^2$	$z_{22} = c^8 + 14(c^2s^6 - c^6s^2) - s^8 + 6i(c^7s + cs^7) - 14i(c^5s^3 + c^3s^5)$
$r_{25} = \sqrt{140}(c^3s^5 - c^5s^3)$	$z_{33} = c^8 - 4(c^6s^2 + c^2s^6) - 10c^4s^4 + s^8 + 4i(c^7s + c^5s^3 - c^3s^5 - cs^7)$
$r_{26} = \sqrt{175}c^4s^4 - \sqrt{63}c^2s^6$	$z_{44} = c^8 + 2(c^6s^2 - c^2s^6) - s^8 + 2i(c^7s + cs^7) + 6i(c^5s^3 + c^3s^5)$
$r_{27} = \sqrt{126}c^3s^5 - \sqrt{14}cs^7$	$z_{55} = 1$

Conclusions

Spin-based quantum computing uses qubit systems (spin-1/2, single electron or proton), qutrit systems (spin-1, electron pair or nuclei), and qudit systems (spin>1). Present studies on spin-based quantum computation system concentrate mainly on qubit system, but higher spin system also seem to be promising. Besides the nuclei with higher spins, carbon nanotubes or fullerenes may contain two, three or more unpaired electrons therefore, it seems necessary to establish the theoretical foundations of large spin systems. Since EPR spectroscopy can work in different spin systems, it is evident that quantum mechanical spin operators, some basic quantum gates corresponding quantum rotation operators will encourage investigation for spin systems greater than spin-1/2.

Quantum mechanical rotation operators $R_X(\theta)$, $R_Y(\theta)$ and $R_Z(\theta)$ corresponding to spin-4 were formed by series expansion of exponential operator and variations generated for each element of rotation operator were fitted by least squares procedure to linear functions of sines and cosines. The operators $R_X(\theta)$ and $R_Z(\theta)$ in matrix forms are symmetric, and $R_Y(\theta)$ is antisymmetric. The rotation operators found can be used to determine the rotations of the corresponding spins or dipoles around three Cartesian coordinates. It is expected that it can form a basis for its implementation for spin-4 or equivalent magnetic dipole systems.

Conflicts of interest

The authors state that did not have conflict of interests.

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