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Understanding The Ferro-Magnet Electron Spin: Through Matrix Methods

Vandana Arora, Jyoti Anand, Jagneet Kaur Anand
(Department Of Physics, Keshav Mahavidyalaya, University Of Delhi, India)
(Department Of Electronics, Keshav Mahavidyalaya, University Of Delhi, India)

Abstract:
A detailed analysis of the matrix methods is done. The aim is to apply these matrix methods to understand functioning of spintronic devices. We have explored a two-electron composite system in a ferromagnet system. The electron spin has been utilized in various spintronic devices by utilizing FN (Ferromagnet/Non-ferromagnet) junctions. The aim is to increase the efficiency of the spintronic devices by mathematical models.
Key Word: *Matrix methods; Projection matrix; Trace; Spintronics; Electron spin; Ferro-magnet*

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I. Introduction

The matrix methods, such as, the orthonormal bases, Gram-Schmidt process, invertible/reversible matrices, determinants, projections, Eigen Values, Eigen vectors, span, range, rank, square root, reduction map, positive semidefinite (PSD), density matrices, reduced density matrices, Trace, partial trace, and partial transpose are discussed with emphasis on applications in understanding a multiple-electron-spin system in spintronic devices. The case of a two electrons system in a ferromagnetic material is considered discussed utilizing the matrix algebra.

II. Linear And Matrix Algebra: Role In Quantum Computing

The quantum bits (qubits) are designated as the orthonormal bases of a unitary matrix. The mathematical computations involving quantum bits deal with matrices, vector spaces, and tensors. A single qubit is represented as a 2×1 column vector in the ket notation ($|q\rangle$). The orthonormal bases for a composite quantum system (consisting of more than 1 qubit) is obtained by the tensor product (Kronecker product) of the orthonormal bases of the constituent qubits. The difference between orthonormal bases and any linearly independent bases is that orthonormal bases form a unit square grid, whereas any other linearly independent bases form a parallelogram grid (Johnston 2021). In fact, any non-zero invertible matrix converts the unit square grid into parallelogram grid. A matrix which is non-invertible, i.e., with zero determinant will collapse a square or parallelogram grid into a line resulting in loss of information (non-invertible/irreversible). Given any linearly independent bases of a matrix/ vector space/ polynomial, one can always calculate the corresponding orthonormal bases using Gram-Schmidt Process (Denton and Waldron 2012; Johnston 2021; Lipschutz and Lipson 2009).

Determinant of a matrix A can be interpreted as a measurement of expansion of the space occupied by orthonormal bases when operated upon by A. Determinant is generally calculated using the permutation formula. For a diagonal matrix, the determinant is given by the sum of its diagonal elements which is also the definition of Trace of a matrix. Determinant of similarity matrices is the same.

Determinant of a matrix A is a measure of how much a linear transformation (provided by the matrix A) expands or contracts space. Trace can be compared with determinant in providing similar information. Trace of an n-dimensional identity matrix is $trace(I) = n$. If the trace of any matrix C is zero then there must exist matrices A and B such that there commutation $[A, B]$ is given by $AB - BA = C$. Geometric interpretation of Trace tells that if

$f_A: \mathbb{F} \to \mathbb{F}$ (1)
Such that

$f_A = \det(I + xA)$ (2)

Where x is the $x - axis$ space coordinate, then
$f_A' = trace(A)$ (3)

That is, the trace is the directional derivative of the determinant.

Eigen values λ and corresponding Eigen vectors $\boldsymbol{v}$ of a matrix A are computed from the its characteristic equation $\det(A - \lambda I) = p_A(\lambda)$, where I is the identity matrix of same dimensions as matrix A, and $p_A(\lambda)$ is a polynomial in λ, and the degree of p_A is the size of A. The Eigen vectors of A belong to subspace of A called the Eigenspace. One of the applications of Eigen values and Eigen vectors is to diagonalize the corresponding matrix A satisfying the relation $A = PDP^{-1}$, where the Eigen values of A are the diagonal elements in matrix D and the columns of matrix P consist of the corresponding Eigen vectors in the same order. Matrices A and D are similarity matrices, because of the fact that these two matrices (and for that matter, any group of similarity matrices) have same Eigen Values. Trace of similarity matrices is the same. Hence Trace can be evaluated as the sum of Eigen values of a matrix.

Mathematically, we can write the Trace of a square matrix A as the sum of its diagonal terms a_{ii}:

$$Trace(A) = \sum_{i=1}^{n} a_{ii} \quad (4)$$

Trace can also be obtained as the sum of Eigen values of matrix A counted with multiplicities:

$$Trace(A) = \sum_{i=1}^{n} \lambda_i \quad (5)$$

Physical significance of Trace: Trace is not just a mathematical number, in quantum computing it ensures that the probabilities are normalized (Trace of a density matrix $(\boldsymbol{\rho})$ is unity (Blum 2012), Vandana Arora 2025), this will be discussed in detail in later sections in this paper.

$$Trace(\boldsymbol{\rho}) = 1 \quad (6)$$

Trace also gives the expectation value of an observable $\langle x \rangle$ in quantum mechanics:

$$\langle x \rangle = Trace(\boldsymbol{\rho} x) \quad (7)$$

In physics, Trace is linked to flux, pressure, and stress tensors, giving a 'total sum' of the effect of any matrix.

Let us now understand the terms: span, range, and rank of a matrix. 'Span' is the set of all the vectors one can make in a given vector space, or a matrix of a given dimension. 'Range' gives the span of all the columns in a given matrix. And 'rank' tells the dimension of the range, *i.e.* the number of independent columns of a matrix.

Square root of a matrix: If matrix B is the square root of matrix A, then

$$B^2 = A \quad (8)$$

Not every matrix has a real square root, but every positive semi-definitive matrix does have a real square root. The square root of a matrix is not unique, meaning that there can be multiple square root matrices corresponding to a matrix. Square root matrix does have a physical significance: in quantum mechanics, the density matrix $\boldsymbol{\rho}$ can be written as $\boldsymbol{\rho} = \sqrt{\boldsymbol{\rho}}\sqrt{\boldsymbol{\rho}}$. The density matrix describes the mixed states, and its square root appears in defining the **purifications** of mixed states (embedding the system in a larger Hilbert space). Also in measurement probabilities $p(i) = Trace(M_i^{\dagger} M_i \boldsymbol{\rho})$, the M_i operators are usually constructed from the square root of positive operators. For example, in quantum mechanics, when making a measurement using computational bases E_i , the probability of outcome i when measuring a state $\boldsymbol{\rho}$ is:

$$p(i) = Trace(E_i \boldsymbol{\rho}) \quad (9)$$

In order to connect this to the 'state update rule' after measurements, *i.e.* the state collapses to i after measurement outcome reveals i state; we introduce measurement operator M_i such that

$$E_i = M_i^{\dagger} M_i \quad (10)$$

This guarantees that E_i is positive semidefinite (PSD), *i.e.* the probabilities are consistent (non-negative):

$$p(i) = Trace(M_i^{\dagger} M_i \boldsymbol{\rho}) \quad (11)$$

Now if after the measurement, the outcome state is i , then state of the system collapses to

$$\boldsymbol{\rho} \mapsto \frac{M_i \boldsymbol{\rho} M_i^\dagger}{p(i)} \tag{12}$$

Projection (P) can be thought of as a linear transformation that crushes the vectors when operated upon, onto a sub-space of the original vector space. For a given sub-space of a vector-space, there is a unique orthogonal projection, whereas there are numerous oblique projections for the same sub-space. Making a projection twice has no additional effect over a single projection, hence $P^2 = P$. An orthogonal projection matrix is symmetric about the main diagonal. The trace of a projection matrix is the same as its rank, in other words, it tells about the dimension of the subspace projected onto by the projection matrix P.

The next important linear mapping in matrices is the "Reduction Map" Φ_R: $\mathrm{M}_n \to \mathrm{M}_n$, which is defined as

$$\Phi_R(X) = Trace(X)I - X \tag{13}$$

The reduction map takes a matrix X, and subtracts it from a multiple of the identity equal to its trace. It can be shown that the reduction map neatly separates the trace part from the traceless part. In quantum theory, the reduction map plays two important roles: detection of entanglement, and to highlight the "trace component" vs. "traceless component" structure of an operator, which is crucial for understanding quantum state decompositions.

With all the basic terms now understood about matrix algebra, we will now focus on to their applications in understanding the quantum computation terms, such as, density matrix, reduced density matrix, and partial trace.

The density matrix $\boldsymbol{\rho}$ corresponding to a quantum state |φ⟩ (pure or mixed) is calculated as the outer product of the quantum state with itself, *i.e.* $\boldsymbol{\rho} = |\varphi\rangle\langle\varphi|$. The physical interpretation of density matrix is that the diagonal terms give the probability density of the quantum state $|\varphi\rangle$ in the computational bases and its trace is equal to unity signifying that the total probability of occurrence of $|\varphi\rangle$ is unity. The off-diagonal terms are related to the entanglement.

By calculating partial trace and partial transpose on the density matrix, the details of the entanglement can be evaluated. The **partial trace** is how to "ignore" or "discard" part of a bipartite quantum system consisting of two quantum states |A⟩and |B⟩. Let the density matrix of the bipartite system is

$$\boldsymbol{\rho_{AB}} = \mathcal{H}_A \otimes \mathcal{H}_B \tag{14}$$

The reduced density matrix of sub-system A by taking partial trace over sub-system B is evaluated as:

$$\boldsymbol{\rho_A} = Trace_B(\boldsymbol{\rho_{AB}}) \tag{15}$$

The trace of $\boldsymbol{\rho_{AB}^2}$ is unity ($Trace\left(\boldsymbol{\rho_{AB}^2}\right) = 1$), whereas the value of the partial trace of reduced matrix gives a measure of the entanglement of the sub-systems A and B. For example, for a Bell state, which is maximally entangled, and the partial trace can be shown to be $Trace\left(\boldsymbol{\rho_A^2}\right) = Trace\left(\frac{1}{2}I\right) = \frac{1}{2} < 1$. It is emphasized here that Trace is a scalar quantity, whereas partial Trace is an operator function.

Partial Transpose: The **partial transpose** is an operation where *only one subsystem* of a bipartite operator is transposed. According to the **Peres–Horodecki criterion (PPT test)**:

if $\boldsymbol{\rho_{AB}}$ is separable, *i.e.* consists of mixed states, then partial transpose of $\boldsymbol{\rho_{AB}}$, *i.e.* $\boldsymbol{\rho}_{AB}^{T_B} \geqslant 0$ (positive semidefinite, PSD)
And if $\boldsymbol{\rho}_{AB}^{T_B}$ has negative Eigen values, then $\boldsymbol{\rho_{AB}}$ is entangled.

III. Electron Spin Relaxation Process

The pillar of spintronic devices is an FN (Ferromagnetic/Non-ferromagnetic) junction. Materials with ferromagnetic/anti-ferromagnetic properties include Fe, Ni, Co, Fe_3O_4, CrO_2, to name a few. The polarized spin electrons are injected from F-region to N-region, where their spins start to relax (de-polarize) away from the FN interface due to various relaxation mechanisms such as, the "spin-orbit interaction", "Hyperfine lines", "carrier-carrier interaction", "environment interaction" (Dey and Roy 2021), resulting in alterations in their orientations.

In this paper, we consider a system of two electrons in a ferromagnetic material and evaluate the spin relaxation mechanisms using Pauli's matrix algebra. For a spin $\frac{1}{2}$ particle, the spin operator is given as:

$$\widehat{\boldsymbol{S}} = \frac{\hbar}{2}\boldsymbol{\sigma} \tag{16}$$

Where $\boldsymbol{\sigma} = (\boldsymbol{\sigma_x}, \boldsymbol{\sigma_y}, \boldsymbol{\sigma_z})$ are the Pauli's matrices, given by:

$$\boldsymbol{\sigma_x} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \tag{17}$$

$$\boldsymbol{\sigma_y} = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \tag{18}$$

$$\boldsymbol{\sigma_z} = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \tag{19}$$

The corresponding spin operators are $\widehat{\boldsymbol{S_x}} = \frac{\hbar}{2}\boldsymbol{\sigma_x}$, $\widehat{\boldsymbol{S_y}} = \frac{\hbar}{2}\boldsymbol{\sigma_y}$, $\widehat{\boldsymbol{S_z}} = \frac{\hbar}{2}\boldsymbol{\sigma_z}$. For an N-aligned spins in a ferromagnet, the total spin operator is given as

$$\widehat{\boldsymbol{S}}_{\boldsymbol{Total}} = \sum_{\boldsymbol{i=1}}^{\boldsymbol{N}} \widehat{\boldsymbol{S}}_{\boldsymbol{i}} \tag{20}$$

In case of fully polarized N ground states, the giant spin is given by $\boldsymbol{S} = \frac{N}{2}$ and the spin matrix is now $(2S+1) \times (2S+1)$ dimensions instead of 2×2 Pauli matrices. The actual magnetization direction of the composite system is encoded in the expectation value of this $(2S+1) \times (2S+1)$ matrix.

For two-electron composite system, the total spin operator is obtained as:

$$\widehat{\boldsymbol{S}}_{\boldsymbol{x}} = \frac{\hbar}{2}(\boldsymbol{\sigma_x} \otimes \boldsymbol{I} + \boldsymbol{I} \otimes \boldsymbol{\sigma_x}) = \frac{\hbar}{2}\begin{pmatrix} 0 & 1 & 1 & 0 \\ 1 & 0 & 0 & 1 \\ 1 & 0 & 0 & 1 \\ 0 & 1 & 1 & 0 \end{pmatrix} \tag{21}$$

$$\widehat{\boldsymbol{S}}_{\boldsymbol{y}} = \frac{\hbar}{2}(\boldsymbol{\sigma_y} \otimes \boldsymbol{I} + \boldsymbol{I} \otimes \boldsymbol{\sigma_y}) = \frac{\hbar}{2}\begin{pmatrix} 0 & -i & -i & 0 \\ i & 0 & 0 & -i \\ i & 0 & 0 & -i \\ 0 & i & i & 0 \end{pmatrix} \tag{21}$$

$$\widehat{\boldsymbol{S}}_{\boldsymbol{z}} = \frac{\hbar}{2}(\boldsymbol{\sigma_z} \otimes \boldsymbol{I} + \boldsymbol{I} \otimes \boldsymbol{\sigma_z}) = \frac{\hbar}{2}\begin{pmatrix} 2 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -2 \end{pmatrix} \tag{21}$$

The square of the total spin is evaluated as follows:

$$\widehat{\boldsymbol{S}}^{\boldsymbol{2}}_{\boldsymbol{Total}} = \widehat{\boldsymbol{S}}^{\boldsymbol{2}}_{\boldsymbol{x}} + \widehat{\boldsymbol{S}}^{\boldsymbol{2}}_{\boldsymbol{y}} + \widehat{\boldsymbol{S}}^{\boldsymbol{2}}_{\boldsymbol{z}} = \begin{pmatrix} 2\hbar^2 & 0 & 0 & 0 \\ 0 & \hbar^2 & \hbar^2 & 0 \\ 0 & \hbar^2 & \hbar^2 & 0 \\ 0 & 0 & 0 & 2\hbar^2 \end{pmatrix} \tag{22}$$

Density Matrices:

A simple ferromagnet example consists of pure fully polarized state, *i.e.* both spins up. Take the pure state as:

$$|\varphi\rangle = |00\rangle = |0\rangle\langle 0| \tag{23}$$

The corresponding density matrix is

$$\boldsymbol{\rho_{00}} = |00\rangle\langle 00| = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \tag{24}$$

The corresponding single-spin reduced matrix is:

$$\boldsymbol{\rho}^{(1)} = \boldsymbol{Tr_2}(\boldsymbol{\rho_{00}}) = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} = |0\rangle\langle 0| \tag{25}$$

($\boldsymbol{Tr_2}$ implies tracing out spin 2)

Eqn. 25 concludes that each spin is in pure state $|0\rangle$ which is expected for a fully polarized pair.

Now considering the case when the density matrix projects onto a triplet sub-space of the ferromagnet, let the system be in an unpolarized state within the triplet manifold:

$$\boldsymbol{\rho_{triplet}} = \frac{1}{3}\sum_{m=+1,0,-1} |1,m\rangle\langle 1,m| = \begin{pmatrix} \frac{1}{3} & 0 & 0 & 0 \\ 0 & \frac{1}{6} & \frac{1}{6} & 0 \\ 0 & \frac{1}{6} & \frac{1}{6} & 0 \\ 0 & 0 & 0 & \frac{1}{3} \end{pmatrix} \tag{26}$$

Its single-spin reduced density matrix (tracing out the second spin) is obtained as

$$\boldsymbol{Tr_2}\left(\boldsymbol{\rho_{triplet}}\right) = \frac{\mathbf{1}}{\mathbf{2}}\boldsymbol{I_{(2\times 2)}} = \begin{pmatrix} \frac{1}{2} & 0 \\ 0 & \frac{1}{2} \end{pmatrix} \tag{27}$$

Eqn. 27 can be interpreted as the two-spin system in a triplet manifold has no information about the orientation, each individual spin is maximally mixed, *i.e.* completely unpolarized, and has a reduced state as $\frac{1}{2}I$.

IV. Discussion

The authors have given a detailed description of the matrix algebra required to understand the quantum nature of electron spin in spintronic devices. A two-electron pure and triplet states of a ferromagnet is analyzed using the methods of the density matrix. Reduced density matrices are computed using partial tracing technique. The mathematical model is verified in a real spintronic environment.

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