EAST EUROPEAN JOURNAL OF PHYSICS. 4. 87–100 (2025)
DOI: 10.26565/2312-4334-2025-4-08 ISSN 2312-4334

SPIN ALGEBRA AND NAIMARK'S EXTENSION: A TUTORIAL APPROACH WITH EXAMPLES

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Received August 12, 2025; revised October 10, 2025; accepted November 10, 2025

In analyzing two-electron systems, the interactions of interest often include the spin-spin operator $\vec{S}_1 \cdot \vec{S}_2$ and the spin-orbit operator $\vec{L} \cdot \vec{S}$. When these operators act on entangled or indistinguishable particles, their measurement and physical interpretation may extend beyond the standard projective framework. This tutorial introduces the algebraic structure of spin interactions in two electron quantum systems and establishes its conceptual and mathematical connection with *Naimark's Extension Theorem*. Through explicit examples for two-electron systems, we demonstrate how spin operators arise in reduced Hilbert spaces, and how *Naimark's theorem* provides a formal framework for extending them to projective measurements in enlarged spaces. The application of *Naimark's Extension Theorem* in deriving their matrix elements opens up a window into the structure of quantum measurements in such composite systems.

Keywords: *Naimark's Extension; Hilbert space; Lie Algebra; Breit Hamiltonian; Quantum computing*

PACS: 03.65.-w;03.65.Fd;03.65.Ta;03.65.Ca;03.67.-a

1. INTRODUCTION

In quantum mechanics, spin is an intrinsic form of angular momentum, described by the $\mathfrak{su}(2)$ Lie algebra. In multi-electron systems, interactions like spin-spin and spin-orbit couplings are fundamental in determining spectral structures and quantum correlations. However, when systems are not fully accessible or are entangled with external degrees of freedom, effective descriptions via Positive Operator-Valued Measures(POVMs) often arise. *Naimark's Extension Theorem*[1-4,14, 15, 18-21] bridges this gap by ensuring that any POVM can be viewed as a Projection-Valued Measure(PVM) in a higher-dimensional Hilbert space. This article builds an intuitive and formal connection between spin algebra and Naimark's extension, with physically motivated examples. This paper calculates all the matrix elements associated with the spin-spin and spin-orbit operators for helium-like systems (He, Li^+) using an algebraic method, comparing the results with the conventional quantum mechanical calculations by G. Araki[5-7]. The spin-algebraic approach simplifies traditional quantum mechanics using tensor algebra and offers potential applications in quantum computing. We connect this algebraic approach to quantum mechanics foundations such as Dirac's vector space framework and the algebra of finite matrices[8].

This paper is organized as follows: Section 1 provides an introduction to spin algebra. Section 2 Naimark Extension theorem and other associated theories related to spin algebra. In Section 3, we outline the algebraic theories related to spin algebra. In section 4 we present the detailed calculations of the spin-dependent terms in the Breit Hamiltonian, highlighting our main results related to spin-spin and spin-orbit interactions. Section 5 establishes the connection between spin algebra and quantum computing theory. In Section 6, we summarize our analytical findings and discuss their consistency with previously reported results. Finally, Section 7 outlines potential future directions and concludes the paper.

Our results, compared with previous work, form a basis for developing quantum algorithms and logic gates, with plans to incorporate silicon-based calculations in future work. This research aims to explore the advantages of quantum computing and develop strategies for error correction and improved device performance, ultimately contributing to the realization of fault-tolerant quantum computers.

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Cite as: S. Datta, East Eur. J. Phys. 4, 87 (2025), https://doi.org/10.26565/2312-4334-2025-4-08

This paper is organized as follows: Section 1 provides an introduction to spin algebra. Section 2 delves into the Naimark Extension theorem and other associated theories related to spin algebra. In Section 3, we outline the algebraic theories related to spin algebra. In section 4 we present the detailed calculations of the spin-dependent terms in the Breit Hamiltonian, highlighting our main results related to spin-spin and spin-orbit interactions. Section 5 establishes the connection between spin algebra and quantum computing theory. In Section 6, we summarize our analytical findings and discuss their consistency with previously reported results. Finally, Section 7 outlines potential future directions and concludes the paper.

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2. NAIMARK'S EXTENSION AND GENERALIZED MEASUREMENTS

Naimark's Extension Theorem states that for any POVM $\{E_i\}$ acting on a Hilbert space $\mathcal{H}$, there exists a larger Hilbert space $\mathcal{K} \supset \mathcal{H}$ and a projective measurement $\{P_i\}$ on $\mathcal{K}$, such that

$$E_i = V^\dagger P_i V,$$

where $V : \mathcal{H} \to \mathcal{K}$ is an isometry. This result allows one to represent generalized (unsharp) measurements as projective (sharp) measurements on an extended system, possibly involving an ancillary system.

2.1. Spin-Spin Interaction as a Measurement of Joint Observables

The spin-spin interaction is described by:

$$\vec{S}_1 \cdot \vec{S}_2 = \frac{1}{2}\left(\vec{S}^2_{\text{tot}} - \vec{S}^2_1 - \vec{S}^2_2\right),$$

which is a function of total spin. Measuring this interaction amounts to resolving joint properties of the two-electron system. However, such joint measurements are not always directly implementable within $\mathcal{H}_1 \otimes \mathcal{H}_2$, especially when the spins are entangled. By extending the Hilbert space via Naimark's theorem, we can model the measurement of $\vec{S}_1 \cdot \vec{S}_2$ as a sharp measurement on a larger space $\mathcal{K}$, where a projective observable P satisfies

$$\langle \psi | \vec{S}_1 \cdot \vec{S}_2 | \psi \rangle = \langle V\psi | P | V\psi \rangle .$$

This realizes the spin-spin operator as a component of a generalized measurement, effectively mediated by an ancilla system or latent degrees of freedom.

2.2. Spin-Orbit Interaction as a Quantum Instrument

The spin-orbit interaction,

$$\vec{L} \cdot \vec{S} = \sum_{i=1}^{3} L_i S_i,$$

entangles spin and orbital angular momenta. It can be viewed as a *quantum instrument*, a device that performs a measurement on one subsystem (e.g., orbital) and conditionally transforms the other (e.g., spin).

Naimark's theorem implies that this transformation may arise from a projective measurement on an extended space involving an ancilla. Mathematically, the spin-orbit coupling operator can be embedded into a larger Hilbert space via:

$$\vec{L} \cdot \vec{S} = V^\dagger \left(\sum_i \tilde{L}_i \tilde{S}_i \right) V,$$

where $\tilde{L}_i$, $\tilde{S}_i$ are extended operators acting on $\mathcal{K}$. This framework enables interpretation of spin-orbit interactions as information flow between degrees of freedom through a measurement process.

2.3. Ancilla Interpretation and Emergent Observables

The embedding via Naimark naturally introduces an ancillary space $\mathcal{A}$, such that:

$$\mathcal{K} = \mathcal{H} \otimes \mathcal{A}.$$

The matrix elements one can derive for spin operators in this framework suggest that some observables—particularly those not simultaneously measurable—can be effectively simulated as projective measurements on this enlarged space. These matrix elements therefore encode emergent properties due to the system-ancilla interaction.

2.4. Theorems and Lemmas Related to Naimark's Extension and Spin Interactions

Definition (POVM): A *positive operator-valued measure* (POVM) on a Hilbert space $\mathcal{H}$ is a set $\{E_i\} \subset \mathcal{B}(\mathcal{H})$ such that:

$$E_i \geq 0 \quad \text{and} \quad \sum_i E_i = \mathbb{I}_{\mathcal{H}}.$$

Theorem 1 (Naimark's Dilation Theorem): Let $\{E_i\}$ be a POVM on a Hilbert space $\mathcal{H}$. Then there exists a larger Hilbert space $\mathcal{K} \supset \mathcal{H}$, an isometry $V : \mathcal{H} \to \mathcal{K}$, and a projection-valued measure (PVM) $\{P_i\}$ on $\mathcal{K}$ such that

$$E_i = V^\dagger P_i V.$$

This theorem allows generalized spin measurements (e.g., effective measurement of $\vec{S}_1 \cdot \vec{S}_2$) to be implemented via sharp measurements on an extended Hilbert space.

Lemma 1 (Operator Realization via Ancilla): Let $A \in \mathcal{B}(\mathcal{H})$ be a Hermitian operator that does not correspond to a measurable quantity in the standard sense (e.g., $\vec{L} \cdot \vec{S}$, when spin and orbital observables are not jointly measurable). Then there exists an ancilla Hilbert space $\mathcal{A}$ and a Hermitian operator $\tilde{A} \in \mathcal{B}(\mathcal{H} \otimes \mathcal{A})$ such that

$$\langle\psi|A|\psi\rangle = \langle\psi \otimes \eta|\tilde{A}|\psi \otimes \eta\rangle, \quad \forall\psi \in \mathcal{H},$$

where $\eta \in \mathcal{A}$ is a fixed ancilla state. This lemma provides a foundation for calculating matrix elements of spin-orbit operators via auxiliary systems.

Theorem 2 (Joint Measurement Representation): Let $A, B \in \mathcal{B}(\mathcal{H})$ be two noncommuting observables (e.g., spin components or spin-orbit coupled operators). Then there exists a POVM $\{E_{ij}\}$ on $\mathcal{H}$ that approximates a joint measurement of A and B, and an extended Hilbert space $\mathcal{K} \supset \mathcal{H}$ such that:

$$E_{ij} = V^\dagger P_{ij} V, \quad \text{with } \{P_{ij}\} \text{ a PVM on } \mathcal{K}.$$

This allows one to interpret the joint statistics of $\vec{S}_1 \cdot \vec{S}_2$ and $\vec{L} \cdot \vec{S}$ in terms of projective measurements in an enlarged space.

Lemma 2 (Matrix Element Preservation): Let $A \in \mathcal{B}(\mathcal{H})$ be an observable and $\tilde{A} \in \mathcal{B}(\mathcal{K})$ be its Naimark extension such that $A = V^\dagger \tilde{A} V$. Then for any $\psi, \phi \in \mathcal{H}$,

$$\langle\psi|A|\phi\rangle = \langle V\psi|\tilde{A}|V\phi\rangle.$$

Hence, matrix elements of spin-spin or spin-orbit operators derived via an extended space are consistent with those computed in the physical Hilbert space using POVM descriptions.

Corollary (Simulation of Noncommuting Observables): Spin observables that cannot be simultaneously diagonalized (e.g., S_x, S_y) can still be jointly simulated via projective measurements in an extended space, consistent with quantum contextuality. This supports the derivation of matrix elements for spin-spin and spin-orbit interactions via the Naimark formalism.

2.5. Quantum Information Perspective

From a quantum information viewpoint, this formalism is closely related to:

- **Entanglement-assisted measurements:** where outcomes depend on entangled ancillae.
- **Measurement-based quantum computation:** where operations are simulated via measurement on entangled states.
- **Contextuality and non-locality:** since the need for extensions often stems from non-classical statistics of spin observables.

3. QUANTUM SPIN SYSTEMS

Quantum spin systems[16] arise when the Hilbert space of states of atoms and molecules are reduced to a finite dimensional subspace. Here in this paper we consider the 2- particle quantum spin system, namely a helium atom with two spin-half electrons. To describe spin states of 2-electrons inside a helium atom, we consider a finite dimensional complex space called Hilbert space $\mathcal{H} = C^2$.

3.1. Postulates of Quantum Mechanics

1) The state of a particle in the quantum system is represented by a state vector in the Hilbert space. One can get all the information about the system by looking at the state vector.

2) The general quantum state of a quantum system is represented by a linear superposition of the individual states.

3) The state evolves by a unitary transformation.

4) All the observables(dynamical measurable variables) of a system can be represented by some operators.

5) The measured value of any physical observable is always real, so the corresponding operators are Hermitian.

3.2. Dirac notations for the state vector

For each state vector, $|\psi >\in \mathcal{H} \ \exists < \chi| \in$ dual space
Bra and ket states: For each $|\psi >$ in linear vector space $\exists$ one $< \psi|$ in dual space. ket vector $|\psi >$ is analogous to ψ in wave mechanics. bra vector $< \psi|$ is analogous to ψ^* in wave mechanics.
Projections: The projectors P_ψ onto a ket. Define $P_\psi = |\psi >< \psi|$ and apply it to an arbitrary ket $|\phi >$; $P_\psi|\phi >= |\psi >< \psi|\phi >$ In both the cases above we have used the concept of Naimark-Segal's extension formula[1-4, 14, 15,18-21].

3.3. Algebra of the spin groups

An algebra is a vector space equipped with bilinear operations. Algebra $\mathcal{A}$ of observables of a quantum system is the set of all bounded operators on $\mathcal{H}$, denoted by $\mathcal{B}(\mathcal{H})$

3.3.1. Lie Group A Lie group[22-25] G with a compatible structure of a smooth (real or complex) manifold, in which the group operations of multiplication and inversion are smooth maps. Or in other words
if $\mu : G \times G \rightarrow G, \mu(x, y) = xy$, then μ is a smooth map. The spin operators in $\mathcal{H} = C^2$ form a Lie group. The spin groups of $\frac{1}{2}$ integer spin particles are represented by $SU(2)$ whereas the rotation groups in 3D are designated by $SO(3)$. $SU(n)$ and $SO(n)$ are in general defined as:
$SO(n) = \{A \in GL(n, \mathbb{R}) : AA^t = \mathbb{1} \quad \text{and} \quad det(A) = 1\}$
$SU(n) = \{A \in GL(n, \mathbb{C}) : AA^* = \mathbb{1} \quad \text{and} \quad det(A) = 1\}$
These two groups are isomorphic locally and their Lie Algebras are the same. $SU(2)$ is the universal double covering group of $SO(3)$.

The Hermitian generators of $SU(2)$ take the following form: $[\hat{T}_i, \hat{T}_j] = i\epsilon_{ijk}\hat{T}_k$ where $\hat{T}_i = \frac{1}{2}\hat{\sigma}_i$ and $\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$ $\sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$ $\sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$.

3.3.2. Lie Algebra of spin groups If G is a Lie group , then the Lie algebra g associated to G is, $T_{\mathbb{1}}(G)$ i.e., the tangent space of G at the identity $\mathbb{1} \in G$. A Lie algebra g is a special case where bilinear operation behaves like a commutator, in particular the bilinear operations need to satisfy
$[\cdot, \cdot] : g \times g = g$
$[x, x] = 0 \forall x \in g(alternatively)$
$[x, [y, z]] + [y, [z, x]] + [z, [x, y]] = 0 \forall x, y, z \in g$ (Jacobi identity)
$[x, y] + [y, x] = 0 \forall x, y \in g(anticommutivity)$
The Lie algebra associated with $SO(3)$ takes the following form: $[\hat{J}_i, \hat{J}_j] = \epsilon_{ijk}\hat{J}_k$

3.4. Representation of Lie Groups and Lie Algebras connected to spin observables

Let G be a Lie group and W be a finite dimensional vector space over a field $\mathbb{K} \in \{\mathbb{R}, \mathbb{C}\}$. A representation Π of G acting on W is a mapping $\Pi : G \rightarrow GL(W)$ which satisfies
$\Pi(g_1 g_2) = \Pi(g_1)\Pi(g_2) \quad \forall g_1, g_2 \in G \quad$ and $dim(\Pi) = dim(V)$ If g be a Lie Algebra of the above Lie group G, then a representation π acting on W is a mapping $\pi : g \rightarrow L(W)$ which satisfies
$\pi(|x, y|) = [\pi(x), \pi(y)] \quad \forall x, y \in g \quad$ and $dim(\pi) = dim(W)$. In general, the tensor product of $su(2)$ representations with spin s_1 and s_2 can be written as a fusion rule
$(s_1) \otimes (s_2) = \sum_{s=|s_1-s_2|}^{s_1+s_2}(s)$. For $s_1 = s_2 = \frac{1}{2}$, the decomposition of the Hilbert space can be given as
$(1/2) \otimes (1/2) = (0) + (1)$.

For two spin-(1/2) particles the four states of the Hilbert space can be decomposed into the triplet and the singlet states.
triplet:$|\uparrow\uparrow>, \frac{1}{\sqrt{2}}(|\uparrow\downarrow> + |\downarrow\uparrow>), |\downarrow\downarrow>$
singlet: $\frac{1}{\sqrt{2}}(|\uparrow\downarrow> - |\downarrow\uparrow>)$.

3.5. Naimark's Extension Theorem and Spin Couplings

Naimark's extension theorem provides a deep mathematical and physical insight into the representation of generalized, or unsharp, measurements as projective (sharp) measurements on an enlarged Hilbert space. This idea has a natural and elegant interpretation in the algebra of spin systems, where coupling between subsystems can be seen as an embedding of one Hilbert space into a larger one, typically involving an ancillary degree of freedom.

3.5.1. The statement of Naimark's theorem Let $\mathcal{H}$ be a Hilbert space describing our physical system. A Positive Operator-Valued Measure (POVM) $\{E_i\}$ on $\mathcal{H}$ is a set of positive operators satisfying $\sum_i E_i = I$. Naimark's theorem states that any such POVM can be realized as a projective measurement on a larger space $\mathcal{H}_{\text{ext}} = \mathcal{H} \otimes \mathcal{H}_{\text{anc}}$, where $\mathcal{H}_{\text{anc}}$ is an ancillary Hilbert space, and there exists an isometry

$$V : \mathcal{H} \longrightarrow \mathcal{H} \otimes \mathcal{H}_{\text{anc}}$$

such that

$$E_i = V^\dagger P_i V,$$

where $\{P_i\}$ are projection operators acting on $\mathcal{H}_{\text{ext}}$.

Physically, the embedding V represents the process of coupling the system to an ancilla, performing a sharp measurement on the composite system, and then projecting back to the original space.

3.5.2. Spin-Orbit coupling as a Naimark extension Consider a single electron in an atom, such as helium. Its Hilbert space is a tensor product of an orbital part and a spin part,

$$\mathcal{H} = \mathcal{H}_L \otimes \mathcal{H}_S,$$

where $\mathcal{H}_L$ carries the orbital angular momentum $\mathbf{L}$, and $\mathcal{H}_S$ carries the intrinsic spin $\mathbf{S}$.

The spin–orbit coupling operator is given by

$$\mathbf{L} \cdot \mathbf{S} = L_x S_x + L_y S_y + L_z S_z.$$

If one considers the orbital part alone as the "system" Hilbert space, the influence of the spin degree of freedom makes $\mathbf{L} \cdot \mathbf{S}$ appear as a non-projective, or unsharp, operator on $\mathcal{H}_L$. According to Naimark's theorem, it can be realized as a sharp observable on the extended space $\mathcal{H}_L \otimes \mathcal{H}_S$:

$$\mathbf{L} \cdot \mathbf{S} = V^\dagger \left(\sum_i \tilde{L}_i \tilde{S}_i \right) V.$$

Here the ancilla is the spin Hilbert space $\mathcal{H}_S$, and V is an isometric embedding

$$V : \mathcal{H}_L \to \mathcal{H}_L \otimes \mathcal{H}_S,$$

given explicitly by the Clebsch–Gordan transformation:

$$V|l, m_l\rangle = \sum_{m_s} C^{j\, m_j}_{l\, m_l\, \frac{1}{2}\, m_s} \, |l, m_l\rangle \otimes |\tfrac{1}{2}, m_s\rangle,$$

where $C^{j\, m_j}_{l\, m_l\, \frac{1}{2}\, m_s}$ are the Clebsch–Gordan coefficients connecting orbital and spin states to total angular momentum eigenstates.

In this sense, the spin degree of freedom acts as the *ancilla* that sharpens the unsharp orbital observable into a well-defined total angular momentum observable.

3.5.3. Spin-Spin coupling as a Naimark extension For a two-electron system (as in helium), each electron possesses a spin-$\frac{1}{2}$ degree of freedom. The combined spin space is

$$\mathcal{H}_S = \mathcal{H}_{S_1} \otimes \mathcal{H}_{S_2}.$$

The spin–spin coupling operator is

$$\mathbf{S}_1 \cdot \mathbf{S}_2 = S_{1x} S_{2x} + S_{1y} S_{2y} + S_{1z} S_{2z}.$$

If one wishes to represent $\mathbf{S}_1 \cdot \mathbf{S}_2$ as a projective measurement on an enlarged space starting from $\mathcal{H}_{S_1}$ alone, then the ancilla is naturally the spin space of the second electron, $\mathcal{H}_{S_2}$. Thus,

$$\mathbf{S}_1 \cdot \mathbf{S}_2 = V^\dagger \left(\sum_i \tilde{S}_{1i} \tilde{S}_{2i} \right) V,$$

where

$$V : \mathcal{H}_{S_1} \to \mathcal{H}_{S_1} \otimes \mathcal{H}_{S_2}$$

is again a Clebsch–Gordan embedding mapping single-spin states to the joint singlet-triplet basis:

$$V|\uparrow\rangle = |\uparrow\uparrow\rangle,$$
$$V|\downarrow\rangle = \frac{1}{\sqrt{2}}\big(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle\big),$$

depending on the total spin sector considered.

Hence, $\mathcal{H}_{S_2}$ plays the role of an ancilla that extends the space of one spin to the composite two-spin space where $\mathbf{S}_1 \cdot \mathbf{S}_2$ is a sharp observable.

3.5.4. Summary

Operator	System	Ancilla	Embedding V
$\mathbf{L}\cdot\mathbf{S}$	Orbital space $\mathcal{H}_L$	Spin space $\mathcal{H}_S$	Clebsch–Gordan map
$\mathbf{S}_1\cdot\mathbf{S}_2$	One-spin space $\mathcal{H}_{S_1}$	Second spin $\mathcal{H}_{S_2}$	Clebsch–Gordan map

In both cases, Naimark's extension theorem offers a unified perspective: an apparently unsharp or subsystem-dependent observable (such as $\mathbf{L}\cdot\mathbf{S}$ or $\mathbf{S_1}\cdot\mathbf{S_2}$) becomes sharp when lifted to an extended Hilbert space that includes the appropriate ancilla. The isometry V implementing this lifting is physically realized by the Clebsch–Gordan transformation that couples angular momenta into total angular momentum eigenstates.

3.6. Lie Group and Spin Algebra Connection

The algebra of spin operators is most naturally understood in the framework of Lie groups and their representations. The operators **L**, **S**, and $\mathbf{J}=\mathbf{L}+\mathbf{S}$ are all generators of unitary representations of the Lie group $SU(2)$, whose associated Lie algebra is $su(2)$. This formalism provides a unifying language for understanding spin–orbit and spin–spin couplings as scalar invariants of tensor product representations.

3.6.1. The $su(2)$ Lie algebra The Lie algebra $su(2)$ is generated by the operators $\{S_x, S_y, S_z\}$ satisfying the commutation relations

$$[S_i, S_j] = i\hbar\epsilon_{ijk}S_k,$$

where ϵ_{ijk} is the Levi-Civita symbol. The Casimir operator

$$S^2 = S_x^2 + S_y^2 + S_z^2$$

commutes with all the generators of the algebra, and its eigenvalues classify the irreducible representations (irreps) of $su(2)$:

$$S^2|s, m_s\rangle = \hbar^2 s(s+1)|s, m_s\rangle.$$

The corresponding group $SU(2)$ consists of unitary operators

$$U(\boldsymbol{\theta}) = e^{-i\boldsymbol{\theta}\cdot\mathbf{S}/\hbar},$$

which represent spatial rotations on the Hilbert space of spin states.

3.6.2. Tensor product representations and coupling of spins When two angular momenta are present, such as **L** and **S** or $\mathbf{S}_1$ and $\mathbf{S}_2$, each provides an independent representation of $su(2)$. The combined system is described by the tensor product representation

$$D^{(l)} \otimes D^{(s)} = \bigoplus_{j=|l-s|}^{l+s} D^{(j)},$$

where $D^{(j)}$ are the irreducible representations of $SU(2)$. The map that implements this decomposition is the *Clebsch–Gordan transformation*,

$$V : \mathcal{H}_L \otimes \mathcal{H}_S \longrightarrow \bigoplus_j \mathcal{H}_j,$$

which is also the isometric embedding used in Naimark's extension theorem. The operator V intertwines between representations, satisfying

$$V\, U_L(g) \otimes U_S(g) = U_J(g)\, V,$$

for all $g \in SU(2)$.

3.6.3. Spin–orbit coupling as a Lie algebra scalar The spin–orbit coupling operator

$$\mathbf{L}\cdot\mathbf{S} = L_x S_x + L_y S_y + L_z S_z$$

is a scalar under the diagonal action of $SU(2)$:

$$U(g)\,(\mathbf{L}\cdot\mathbf{S})\,U(g)^\dagger = \mathbf{L}\cdot\mathbf{S}, \quad U(g) = U_L(g) \otimes U_S(g).$$

Therefore, it can be expressed in terms of the Casimir operators of the Lie algebra:

$$\mathbf{L}\cdot\mathbf{S} = \frac{1}{2}(J^2 - L^2 - S^2),$$

where $J^2 = (\mathbf{L}+\mathbf{S})^2$ is the total angular momentum Casimir. This representation emphasizes that $\mathbf{L}\cdot\mathbf{S}$ is an invariant scalar built from the direct product of two $su(2)$ algebras.

3.6.4. Spin–spin coupling as a Lie algebra invariant For a two-electron system, the total spin operator is

$$\mathbf{S} = \mathbf{S}_1 + \mathbf{S}_2,$$

and the spin–spin coupling operator

$$\mathbf{S}_1 \cdot \mathbf{S}_2 = S_{1x}S_{2x} + S_{1y}S_{2y} + S_{1z}S_{2z}$$

can be written analogously as

$$\mathbf{S}_1 \cdot \mathbf{S}_2 = \frac{1}{2}\left(S^2 - S_1^2 - S_2^2\right).$$

Here again, S^2 is the Casimir operator of the total $su(2)$ representation. The eigenvalues of $\mathbf{S}_1 \cdot \mathbf{S}_2$ distinguish the singlet and triplet sectors:

$$\mathbf{S}_1 \cdot \mathbf{S}_2 \,|S = 0\rangle = -\tfrac{1}{4}\hbar^2 \,|S = 0\rangle,$$
$$\mathbf{S}_1 \cdot \mathbf{S}_2 \,|S = 1\rangle = +\tfrac{3}{4}\hbar^2 \,|S = 1\rangle.$$

These correspond to the irreducible representations $D^{(0)}$ and $D^{(1)}$ of $SU(2)$, respectively.

3.6.5. Relation to Naimark's extension From the Lie algebra viewpoint, the Naimark extension operator V introduced earlier can be recognized as an intertwiner between representations of the Lie algebra $su(2)$:

$$L_i \longmapsto \tilde{L}_i = VL_iV^\dagger, \quad S_i \longmapsto \tilde{S}_i = VS_iV^\dagger.$$

The coupling operator in the extended space,

$$\sum_i \tilde{L}_i\tilde{S}_i,$$

is a scalar invariant under the diagonal $SU(2)$ action, and its projection

$$V^\dagger\left(\sum_i \tilde{L}_i\tilde{S}_i\right)V$$

acts as the physical observable on the smaller subsystem. Thus, the embedding of an unsharp observable into a sharp one via Naimark's theorem is fully consistent with the algebraic principle of constructing invariants from coupled $su(2)$ representations.

3.6.6. Tutorial Summary From the perspective of Lie group theory, both spin–orbit and spin–spin interactions arise as scalar invariants of coupled representations of the $su(2)$ Lie algebra. The Clebsch–Gordan map V, which couples two angular momenta into irreducible components, simultaneously serves as the embedding operator in Naimark's extension theorem. Therefore, the Lie algebraic coupling of spins and the measurement-theoretic embedding of unsharp observables are two complementary realizations of the same symmetry structure encoded by the group $SU(2)$.

3.7. Composite systems and Tensor products with Naimark's extension formula

For 1 particle, spin states are defined as $|\uparrow>$ and $|\downarrow>$. For a bipartite system with two electrons(He or Li^+) any operator for the particle 1, $\hat{A}_1 \in \mathcal{H}_1$ ($\mathcal{H}_1$ is known as a complex Hilbert space) can be upgraded to a bigger Hilbert space, $\mathcal{H}_{12}$ by taking the tensor product with the identity operator in $\mathcal{H}_2$ i.e., $\hat{A}_{12} = \hat{A}_1 \otimes \mathbf{I}_2$.
Similarly an operator, $\hat{A}_2 \in \mathcal{H}_2$ is upgraded to $\mathbf{I}_1 \otimes \hat{A}_2$.
Now $(\hat{A}_1) \otimes (\mathbf{I}_2).(\mathbf{I}_1 \otimes \hat{A}_2)(\psi_1 \otimes \psi_2) = \hat{A}_1\psi_1 \otimes \hat{A}_1\psi_2$, where the state vector $\psi_1 \in \mathcal{H}_1$ and the state vector $\psi_2 \in \mathcal{H}_2$.

$$(\hat{A}_1 \otimes \hat{A}_2) \uparrow \otimes \uparrow = (\hat{A}_1 \uparrow) \otimes (\hat{A}_2 \uparrow) \tag{1}$$

The upgradation formula for the addition of spin angular momenta takes the following form:

$$\sigma_+ = (\sigma_{1+} \otimes \mathbf{1} + \mathbf{1} \otimes \sigma_{2+}) \tag{2}$$

In both the cases above we have used the concept of Naimark-Segal's extension formula[1-4,14,15, 18-21].

4. MATRIX ELEMENTS USING NAIMARK'S EXTENSION FORMULA

4.1. Example 1: Spin-spin interaction operators

The operators needed to calculate the relativistic effects are well known. In atomic units with no external electric and magnetic field these are usually written as Eq. (1) of [11]

$$\Delta_r = -\sum_i \frac{\nabla_\mathbf{i}{}^4}{8c^2} + \sum_i \frac{Z\pi}{2c^2}\delta(\mathbf{r_i}) - \sum_{i<j}\frac{\pi}{c^2}\delta(\mathbf{r_i}-\mathbf{r_j}) - \sum_{i<j}\frac{1}{2c^2}\times$$
$$\times\overleftarrow{\nabla}_\mathbf{i}\cdot[\frac{(\mathbf{r_i}-\mathbf{r_j})(\mathbf{r_i}-\mathbf{r_j})}{{r_{ij}}^3} + \frac{1}{r_{ij}}]\cdot\overrightarrow{\nabla}_\mathbf{j} - \sum_{i<j}\frac{8\pi}{3c^2}\delta(\mathbf{r_i}-\mathbf{r_j})\mathbf{s_i}\cdot\mathbf{s_j}$$
$$-\sum_{i<j}\frac{1}{c^2}\mathbf{s_i}\cdot\frac{3(\mathbf{r_i}-\mathbf{r_j})(\mathbf{r_i}-\mathbf{r_j})-{r_{ij}}^2}{{r_{ij}}^5}\cdot\mathbf{s_j} - \sum_i \frac{Z}{2c^2}\frac{1}{r_i^3}\mathbf{s_i}\cdot[\mathbf{r_i}\times i\overrightarrow{\nabla}_\mathbf{i}]$$
$$+\sum_{i\neq j}\frac{1}{c^2}\frac{1}{{r_{ij}}^3}\mathbf{s_i}\cdot[(\mathbf{r_i}-\mathbf{r_j})\times i\overrightarrow{\nabla}_\mathbf{j}] + \sum_{i\neq j}\frac{1}{2c^2}\frac{1}{{r_{ij}}^3}\mathbf{s_j}\cdot[(\mathbf{r_j}-\mathbf{r_i})\times i\overrightarrow{\nabla}_\mathbf{j}], \tag{3}$$

where r_{ij} is the distance between the particles. The first term is the mass velocity correction. The Second and third operators are the electron and nucleus Darwin term respectively. The fourth term is due to the retardation of electromagnetic field by an electron. The fifth and sixth terms represent spin-spin and spin-other spin terms. The last three operators are spin-orbit interactions. For a singlet state with any angular momentum, the expectation values of sixth, seventh and eighth terms are zero. For triplet P and D states, however, the sixth, seventh, eighth and ninth terms are now nonzero and must be computed. Particularly we need to calculate the matrix elements $-\frac{1}{c^2} < \phi|[\Sigma_{i<j}\frac{8\pi}{3}\delta(\mathbf{r_i}-\mathbf{r_j})\mathbf{s_i}.\mathbf{s_j} - \Sigma_{i<j}\mathbf{s_i}.\frac{3(\mathbf{r_i}-\mathbf{r_j})(\mathbf{r_i}-\mathbf{r_j})-{r_{ij}}^2}{{r_{ij}}^5}].\mathbf{s_j}|\phi >$ and $\frac{1}{c^2} < \phi|[\Sigma_{i\neq j}\frac{1}{{r_{ij}}^3}\mathbf{s_i}.[(\mathbf{r_i}-\mathbf{r_j})\times i\nabla_\mathbf{j}] + \Sigma_{i\neq j}\frac{1}{2}\frac{1}{{r_{ij}}^3}\mathbf{s_j}.[(\mathbf{r_j}-\mathbf{r_i})\times i\nabla_\mathbf{j}]|\phi >$
where ϕ is the exact eigenvalue of the unperturbed Hamiltonian.

The spin spin interaction in general for many particle can be written as

$$H_{ss} = 4\mu^2[-\Sigma_{i<j}\frac{8\pi}{3}\delta(\mathbf{r_i}-\mathbf{r_j})[\sigma_\mathbf{i}.\sigma_\mathbf{j} + \frac{1}{{r_{ij}}^3}\{\sigma_\mathbf{i}.\sigma_\mathbf{j} - 3(\sigma_\mathbf{i}.\mathbf{r_{ij}})(\sigma_\mathbf{j}.\mathbf{r_{ij}})/r_{ij}^2] \tag{4}$$

where μ is the Bohr magneton i.e., $\mu = \frac{e\hbar}{2m_e c}$. In atomic units the spin-spin intercation is measured in units of $\frac{1}{c^2}$. For 2 electron system the above expression can be written as[9]

$$\frac{1}{c^2}[-\frac{8\pi}{3}\sigma^\mathbf{1}.\sigma^\mathbf{2}\delta(\mathbf{r_{12}}) + \frac{\mathbf{1}}{\mathbf{r_{12}}^\mathbf{3}}\{\sigma^\mathbf{1}.\sigma^\mathbf{2} - 3(\sigma^\mathbf{1}.\mathbf{r_{12}})(\sigma^\mathbf{2}.\mathbf{r_{12}})/{r_{12}}^2\}] \tag{5}$$

Now since triplet spin function is symmetric $< \delta(r_{12}) >= 0$ for triplet states. So for triplet states only 2nd and third term in Eq (5) contribute.

4.2. Spin states

For 1 particle, spin states are defined as $|\alpha >\equiv |\uparrow>\equiv \begin{pmatrix} 1 \\ 0 \end{pmatrix}$ and $|\beta >\equiv |\downarrow> \equiv \begin{pmatrix} 0 \\ 1 \end{pmatrix}$

For 2 particle systems spin states are defined as $|\alpha_1 > \otimes|\alpha_2 >\equiv |\uparrow> \otimes|\uparrow>$, $|\alpha_1 > \otimes|\beta_2 >\equiv |\uparrow> \otimes|\downarrow>$, $|\beta_1 > \otimes|\alpha_2 >\equiv |\downarrow> \otimes|\uparrow>$ and $|\beta_1 > \otimes|\beta_2 >\equiv |\downarrow> \otimes|\downarrow>$.

4.3. Evaluation of Matrix representation of the spin observables

Using the basis defined in section 4.2, the matrix representation of a general operator R can be represented as

$$\begin{pmatrix} <\uparrow\uparrow|R|\uparrow\uparrow> & <\uparrow\uparrow|R|\uparrow\downarrow> & <\uparrow\uparrow|R|\downarrow\uparrow> & <\uparrow\uparrow|R|\downarrow\downarrow> \\ <\uparrow\downarrow|R|\uparrow\uparrow> & <\uparrow\downarrow|R|\uparrow\downarrow> & <\uparrow\downarrow|R|\downarrow\uparrow> & <\uparrow\downarrow|R|\downarrow\downarrow> \\ <\downarrow\uparrow|R|\uparrow\uparrow> & <\downarrow\uparrow|R|\uparrow\downarrow> & <\downarrow\uparrow|R|\downarrow\uparrow> & <\downarrow\uparrow|R|\downarrow\downarrow> \\ <\downarrow\downarrow|R|\uparrow\uparrow> & <\downarrow\downarrow|R|\uparrow\downarrow> & <\downarrow\downarrow|R|\downarrow\uparrow> & <\downarrow\downarrow|R|\downarrow\downarrow> \end{pmatrix}.$$

We calculate the diagonal matrix elements of the above operator as the correction for the spin spin interaction for triplet states of helium.

4.4. Matrix elements for the spin-spin interactions

Calculation for $(\sigma^\mathbf{1}.\sigma^\mathbf{2})/r_{12}^3$

Let us first calculate $\sigma^1.\sigma^2 = {\sigma_x}^1{\sigma_x}^2 + {\sigma_y}^1{\sigma_y}^2 + {\sigma_z}^1{\sigma_z}^2$

Now

$$\sigma_x{}^1 \otimes \sigma_x{}^2 | \uparrow \otimes \uparrow >= \sigma_x{}^1 | \uparrow > \sigma_x{}^2 | \uparrow > \tag{6}$$

yields
$\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\begin{pmatrix} 1 \\ 0 \end{pmatrix}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\begin{pmatrix} 1 \\ 0 \end{pmatrix}=\begin{pmatrix} 0 \\ 1 \end{pmatrix}\begin{pmatrix} 0 \\ 1 \end{pmatrix}$

$$\sigma_y{}^1 \otimes \sigma_y{}^2 | \uparrow \otimes \uparrow >= \sigma_y{}^1 | \uparrow > \sigma_y{}^2 | \uparrow > \tag{7}$$

yields
$\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}\begin{pmatrix} 1 \\ 0 \end{pmatrix}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}\begin{pmatrix} 1 \\ 0 \end{pmatrix}=\begin{pmatrix} 0 \\ i \end{pmatrix}\begin{pmatrix} 0 \\ i \end{pmatrix}=-\begin{pmatrix} 0 \\ 1 \end{pmatrix}\begin{pmatrix} 0 \\ 1 \end{pmatrix}$

$$\sigma_z{}^1 \otimes \sigma_z{}^2 | \uparrow \otimes \uparrow >= \sigma_z{}^1 | \uparrow > \sigma_z{}^2 | \uparrow > \tag{8}$$

yields
$\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}\begin{pmatrix} 1 \\ 0 \end{pmatrix}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}\begin{pmatrix} 1 \\ 0 \end{pmatrix}=\begin{pmatrix} 1 \\ 0 \end{pmatrix}\begin{pmatrix} 1 \\ 0 \end{pmatrix}$

$$(\sigma^{\mathbf{1}}.\sigma^{\mathbf{2}})/r_{12}^3\begin{pmatrix} \alpha_1\alpha_2 \\ \alpha_1\beta_2 \\ \beta_1\alpha_2 \\ \beta_1\beta_2 \end{pmatrix}=\frac{1}{r_{12}^3}\begin{pmatrix} \downarrow\downarrow - \downarrow\downarrow + \uparrow\uparrow \\ \downarrow\uparrow + \downarrow\uparrow - \uparrow\downarrow \\ \uparrow\downarrow + \uparrow\downarrow - \downarrow\uparrow \\ \uparrow\uparrow - \uparrow\uparrow + \downarrow\downarrow \end{pmatrix}=\frac{1}{r_{12}^3}\begin{pmatrix} \uparrow\uparrow \\ 2\downarrow\uparrow - \uparrow\downarrow \\ 2\uparrow\downarrow - \downarrow\uparrow \\ \downarrow\downarrow \end{pmatrix}$$

Now let us recall $\mathbf{r_{12}} = \mathbf{r} = \hat{i}x + \hat{j}y + \hat{k}z$, where $(x_2 - x_1 = x, y_2 - y_1 = y, z_2 - z_1 = z)$, and $r_{12} = r = \sqrt{(x^2 + y^2 + z^2)}$, where z_1 and z_2 are the z coordinates of electron 1 and 2.

Calculations for $(\sigma^{\mathbf{1}}.\mathbf{r_{12}})(\sigma^{\mathbf{2}}.\mathbf{r_{12}})/r_{12}^5$

$$(\sigma^{\mathbf{1}}.\mathbf{r_{12}})(\sigma^{\mathbf{2}}.\mathbf{r_{12}})/r_{12}^5\begin{pmatrix} \alpha_1\alpha_2 \\ \alpha_1\beta_2 \\ \beta_1\alpha_2 \\ \beta_1\beta_2 \end{pmatrix}$$

Now

$$\begin{aligned}(\sigma^{\mathbf{1}}.\mathbf{r})(\sigma^{\mathbf{2}}.\mathbf{r}) &= (x\sigma_{1x} + y\sigma_{1y} + z\sigma_{1z})(x\sigma_{2x} + y\sigma_{2y} + z\sigma_{2z}) \\ &= x^2\sigma_{1x} \otimes \sigma_{2x} + xy\sigma_{1y} \otimes \sigma_{2x} + xz\sigma_{1z} \otimes \sigma_{2x} + \\ &\quad xy\sigma_{1x} \otimes \sigma_{2y} + y^2\sigma_{1y} \otimes \sigma_{2y} + yz\sigma_{1z} \otimes \sigma_{2y} + \\ &\quad xz\sigma_{1x} \otimes \sigma_{2z} + yz\sigma_{1y} \otimes \sigma_{2z} + z^2\sigma_{1z} \otimes \sigma_{2z}\end{aligned} \tag{9}$$

Now we need to operate $x^2\sigma_{1x} \otimes \sigma_{2x} + xy\sigma_{1y} \otimes \sigma_{2x} + xz\sigma_{1z} \otimes \sigma_{2x} +$
$xy\sigma_{1x} \otimes \sigma_{2y} + y^2\sigma_{1y} \otimes \sigma_{2y} + yz\sigma_{1z} \otimes \sigma_{2y} +$
$xz\sigma_{1x} \otimes \sigma_{2z} + yz\sigma_{1y} \otimes \sigma_{2z} + z^2\sigma_{1z} \otimes \sigma_{2z}$
on $\begin{pmatrix} \alpha_1\alpha_2 \\ \alpha_1\beta_2 \\ \beta_1\alpha_2 \\ \beta_1\beta_2 \end{pmatrix}$.

Operating $x^2\sigma_{1x} \otimes \sigma_{2x} + xy\sigma_{1y} \otimes \sigma_{2x} + xz\sigma_{1z} \otimes \sigma_{2x} +$
$xy\sigma_{1x} \otimes \sigma_{2y} + y^2\sigma_{1y} \otimes \sigma_{2y} + yz\sigma_{1z} \otimes \sigma_{2y} +$
$xz\sigma_{1x} \otimes \sigma_{2z} + yz\sigma_{1y} \otimes \sigma_{2z} + z^2\sigma_{1z} \otimes \sigma_{2z}$
on $\alpha_1\alpha_2$ one gets

$(x + iy)^2\beta_1\beta_2 + (x + iy)z(\alpha_1\beta_2 + \alpha_2\beta_1 + z^2\alpha_1\alpha_2$

Explicit derivation for the above:

Since spin operators are same for particle '1' and particle '2' we suppress the subscript '1' and '2' from now on.

now $\sigma_x=\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$ $\sigma_y=\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$

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

Using the above spin operators we calculate

$$x^2\sigma_x \otimes \sigma_x|\uparrow> \otimes|\uparrow>= x^2\sigma_x|\uparrow> \sigma_x|\uparrow>= x^2 \downarrow\downarrow = x^2\beta_1\beta_2 \tag{10}$$

(we have used $(\hat{A}_1 \otimes \hat{A}_2)|\uparrow> \otimes|\uparrow>= (\hat{A}_1|\uparrow>) \otimes (\hat{A}_2|\uparrow>)$; $\sigma_x|\alpha_1 > \sigma_x|\alpha_2 > =\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\begin{pmatrix} 1 \\ 0 \end{pmatrix}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\begin{pmatrix} 1 \\ 0 \end{pmatrix}=\begin{pmatrix} 0 \\ 1 \end{pmatrix}\begin{pmatrix} 0 \\ 1 \end{pmatrix}$).
Similarly

$$xy\sigma_y \otimes \sigma_x|\uparrow> \otimes|\uparrow>= ixy\beta_1\beta_2, \tag{11}$$

$$xz\sigma_z \otimes \sigma_x|\uparrow> \otimes|\uparrow>= ixz\alpha_1\beta_2, \tag{12}$$

$$xy\sigma_x \otimes \sigma_y|\uparrow> \otimes|\uparrow>= ixy\beta_1\beta_2, \tag{13}$$

$$y^2\sigma_y \otimes \sigma_y|\uparrow> \otimes|\uparrow>= -y^2\beta_1\beta_2, \tag{14}$$

$$yz\sigma_z \otimes \sigma_y|\uparrow> \otimes|\uparrow>= iyz\alpha_1\beta_2, \tag{15}$$

$$xz\sigma_x \otimes \sigma_z|\uparrow> \otimes|\uparrow>= xz\beta_1\alpha_2, \tag{16}$$

$$yz\sigma_y \otimes \sigma_z|\uparrow> \otimes|\uparrow>= iyz\beta_1\alpha_2, \tag{17}$$

$$z^2\sigma_z \otimes \sigma_z|\uparrow> \otimes|\uparrow>= z^2\alpha_1\alpha_2. \tag{18}$$

We have similar relation when we operate

$(\sigma^{\mathbf{1}}.\mathbf{r})(\sigma^{\mathbf{2}}.\mathbf{r})$ on other basis functions. So $(\sigma^{\mathbf{1}}.\mathbf{r_{12}})(\sigma^{\mathbf{2}}.\mathbf{r_{12}})/r_{12}^5 \begin{pmatrix} \alpha_1\alpha_2 \\ \alpha_1\beta_2 \\ \beta_1\alpha_2 \\ \beta_1\beta_2 \end{pmatrix}$

$$=\frac{1}{r_{12}^5}\begin{pmatrix} z^2\alpha_1\alpha_2 + (x+iy)z(\alpha_1\beta_2 + \beta_1\alpha_2) + (x+iy)^2\beta_1\beta_2 \\ z(x-iy)\alpha_1\alpha_2 + (x^2+y^2)\alpha_2\beta_1 - z^2\beta_2\alpha_1 - (x+iy)z\beta_1\beta_2 \\ (x-iy)z\alpha_1\alpha_2 + (x^2+y^2)\beta_2\alpha_1 - z^2\alpha_2\beta_1 - z(x+iy)\beta_1\beta_2 \\ (x-iy)^2\alpha_1\alpha_2 - z(x-iy)(\alpha_1\beta_2 + \beta_1\alpha_2) + z^2\beta_1\beta_2 \end{pmatrix}.$$

Now recalling

$$(\sigma^{\mathbf{1}}.\sigma^{\mathbf{2}})/r_{12}^3 \begin{pmatrix} \alpha_1\alpha_2 \\ \alpha_1\beta_2 \\ \beta_1\alpha_2 \\ \beta_1\beta_2 \end{pmatrix} = \frac{1}{r_{12}{}^3}\begin{pmatrix} \downarrow\downarrow - \downarrow\downarrow + \uparrow\uparrow \\ \downarrow\uparrow + \downarrow\uparrow - \uparrow\downarrow \\ \uparrow\downarrow + \uparrow\downarrow - \downarrow\uparrow \\ \uparrow\uparrow - \uparrow\uparrow + \downarrow\downarrow \end{pmatrix}$$

$$=\frac{1}{r_{12}^3}\begin{pmatrix} \uparrow\uparrow \\ 2\downarrow\uparrow - \uparrow\downarrow \\ 2\uparrow\downarrow - \downarrow\uparrow \\ \downarrow\downarrow \end{pmatrix}.$$

Now taking $R_1 = \frac{1}{r_{12}{}^3}(\sigma^1.\sigma^2) = \frac{1}{r_{12}{}^3}(\sigma_x{}^1\sigma_x{}^2 + \sigma_y{}^1\sigma_y{}^2 + \sigma_z{}^1\sigma_z{}^2)$, the spin average for the second term in Eq. (2) can be calculated by the matrix formula given in section 4.3 as follows:

$$\frac{1}{r_{12}{}^3}\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 2 & 0 \\ 0 & 2 & -1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}.$$

Similarly performing the spin average for the 3rd term, one can get

$$\frac{1}{r_{12}{}^5}\begin{pmatrix} z^2 & (x+iy)z & (x+iy)z & (x+iy)^2 \\ (x-iy)z & -z^2 & (x^2+y^2) & -(x+iy)z \\ (x-iy)z & (x^2+y^2) & -z^2 & -(x+iy)z \\ (x-iy)^2 & -(x-iy)z & -(x-iy)z & z^2 \end{pmatrix}$$

So combining the whole spin spin operator, $(\frac{\sigma^{\mathbf{1}}.\sigma^{\mathbf{2}}}{r_{12}^3} - 3\frac{(\sigma^{\mathbf{1}}.\mathbf{r_{12}})(\sigma^{\mathbf{2}}.\mathbf{r_{12}})}{r_{12}^5})$ using the basis defined in section 3.2, the matrix elements can be represented as $=\begin{pmatrix} \frac{1}{r_{12}{}^3} - \frac{3z^2}{r_{12}{}^5} & -\frac{3(x+iy)z}{r_{12}{}^5} & -\frac{3(x+iy)z}{r_{12}{}^5} & -\frac{3(x+iy)^2}{r_{12}{}^5} \\ -\frac{3(x-iy)z}{r_{12}{}^5} & -(\frac{1}{r_{12}{}^3} - \frac{3z^2}{r_{12}{}^5}) & \frac{2}{r_{12}{}^3} - \frac{3(x^2+y^2)}{r_{12}{}^5} & \frac{3(x+iy)z}{r_{12}{}^5} \\ -\frac{3(x-iy)z}{r_{12}{}^5} & \frac{2}{r_{12}{}^3} - \frac{3(x^2+y^2)}{r_{12}{}^5} & -(\frac{1}{r_{12}{}^3} - \frac{3z^2}{r_{12}{}^5}) & \frac{3(x+iy)z}{r_{12}{}^5} \\ \frac{-3(x-iy)^2}{r_{12}{}^5} & \frac{3(x-iy)z}{r_{12}{}^5} & \frac{3(x-iy)z}{r_{12}{}^5} & \frac{1}{r_{12}{}^3} - \frac{3z^2}{r_{12}{}^5} \end{pmatrix}$

Now the diagonal element of the above matrix is $\frac{1}{r_{12}{}^3} - \frac{3z^2}{r_{12}{}^5}$ which turns out to be $\frac{\partial^2}{\partial z_1 \partial z_2}(\frac{1}{r_{12}})$.

So the diagonal element of the expectation value for the case $(J = L = M)$

$$< LSJM|H_{ss}|LSJM >_{J=L=M}= \frac{1}{4c^2}\int\int |\psi_{LL}|^2 \frac{\partial^2}{\partial z_1 \partial z_2}(\frac{1}{r_{12}})dv_1 dv_2. \tag{19}$$

4.5. Example 2: Spin-orbit operators:

For two particles the spin orbit interaction becomes

$$\frac{1}{4c^2}\{\sigma_1.[\mathcal{E}_1\times p_1+(\frac{2}{r_{12}^3})r_{12}\times p_2]+\sigma_2.[\mathcal{E}_2\times p_2+(\frac{2}{r_{12}^3})r_{21}\times p_1]\}. \tag{20}$$

Now in general $\mathcal{E}=-\nabla V$ includes Coulomb interaction due to the nucleus, the Coulomb interaction due to the other electron and any external field. Since we are not considering any external field, $\mathcal{E}_1$ and $\mathcal{E}_2$ include only the first two interactions. Now $\sigma=\boldsymbol{\sigma_1}+\boldsymbol{\sigma_2}$,
$\boldsymbol{\sigma_1}=\sigma/2+(\boldsymbol{\sigma_1}-\boldsymbol{\sigma_2})/2$. Similarly for $\boldsymbol{\sigma_2}$. Since $\boldsymbol{\sigma_1}$ and σ_2 occur linearly in the H_3, the expectation value of H_3 remains unchanged if $\boldsymbol{\sigma_1}$ and σ_2 are replaced by $\sigma/2$. Making this replacement and putting $\mathcal{E}_1=\frac{zr_1}{r_1{}^3}-\frac{\mathbf{r_{12}}}{r_{12}^3}$ and $\mathcal{E}_2=\frac{zr_2}{r_2{}^3}-\frac{\mathbf{r_{21}}}{r_{21}^3}$, the spin part becomes

$$\frac{1}{4c^2}[\frac{z}{r_1{}^3}\mathbf{r_1}\times\mathbf{p_1}+\frac{z}{r_2{}^3}\mathbf{r_2}\times\mathbf{p_2}+\frac{3}{r_{12}{}^3}(\mathbf{r_1}-\mathbf{r_2})\times(\mathbf{p_1}-\mathbf{p_2})].\sigma \tag{21}$$

$$=\frac{1}{4c^2}[\frac{z}{r_1{}^3}\mathbf{L_1}.\sigma+\frac{z}{r_2{}^3}\mathbf{L_2}.\sigma-\frac{3}{r_{12}{}^3}(\mathbf{L_{12}}+\mathbf{L_{21}}).\sigma]; \tag{22}$$

$$\mathbf{L_1}.\sigma=L_+{}^1\sigma_-+L_-{}^1\sigma_++L_z{}^1\sigma_z, \tag{23}$$

$$\mathbf{L_2}.\sigma=L_+{}^2\sigma_-+L_-{}^2\sigma_++L_z{}^2\sigma_z, \tag{24}$$

$$\mathbf{L_{12}}.\sigma=L_+{}^{12}\sigma_-+L_-{}^{12}\sigma_++L_z{}^{12}\sigma_z, \tag{25}$$

$L_+{}^1=L_x{}^1+iL_y{}^1$, $L_-{}^1=L_x{}^1-iL_y{}^1$.
Now $L_z=\frac{\hbar}{i}\frac{\partial}{\partial\phi}$.
Again,

$$\mathbf{L_1}.\sigma\begin{pmatrix}\chi_{1,1}\\ \chi_{1,0}\\ \chi_{1,-1}\end{pmatrix}=L_+{}^1\sigma_-\begin{pmatrix}\chi_{1,1}\\ \chi_{1,0}\\ \chi_{1,-1}\end{pmatrix}+L_-{}^1\sigma_+\begin{pmatrix}\chi_{1,1}\\ \chi_{1,0}\\ \chi_{1,-1}\end{pmatrix}+L_z{}^1\sigma_z\begin{pmatrix}\chi_{1,1}\\ \chi_{1,0}\\ \chi_{1,-1}\end{pmatrix},$$

$$\sigma_+\begin{pmatrix}\chi_{1,1}\\ \chi_{1,0}\\ \chi_{1,-1}\end{pmatrix}=2\sqrt{2}\begin{pmatrix}0\\ \chi_{1,1}\\ \chi_{1,0}\end{pmatrix},\ \sigma_-\begin{pmatrix}\chi_{1,1}\\ \chi_{1,0}\\ \chi_{1,-1}\end{pmatrix}=2\sqrt{2}\begin{pmatrix}\chi_{1,0}\\ \chi_{1,-1}\\ 0\end{pmatrix},$$

$$\sigma_z\begin{pmatrix}\chi_{1,1}\\ \chi_{1,0}\\ \chi_{1,-1}\end{pmatrix}=2\begin{pmatrix}\chi_{1,1}\\ 0\\ -\chi_{1,-1}\end{pmatrix}$$

The derivation of above transformation relations goes as follows.
$\sigma_\pm=\sigma_{1\pm}+\sigma_{2\pm}$.
Now $\sigma_+=\sigma_{1+}+\sigma_{2+}$.
In the product space

$$\sigma_+=(\sigma_{1+}\otimes\mathbf{1}+\mathbf{1}\otimes\sigma_{2+}) \tag{26}$$

which implies

$$\sigma_+(\uparrow\uparrow)=(\sigma_{1+}\uparrow)\uparrow+\uparrow(\sigma_{2+}\uparrow) \tag{27}$$

$$\begin{pmatrix}0&1\\0&0\end{pmatrix}\begin{pmatrix}1\\0\end{pmatrix}\begin{pmatrix}1\\0\end{pmatrix}+\begin{pmatrix}1\\0\end{pmatrix}\begin{pmatrix}0&1\\0&0\end{pmatrix}\begin{pmatrix}1\\0\end{pmatrix}=0.\begin{pmatrix}1\\0\end{pmatrix}+\begin{pmatrix}1\\0\end{pmatrix}.0=0$$

In the similar manner one can show that
$\sigma_-(\uparrow\uparrow)=2\sqrt{2}\begin{pmatrix}0\\1\end{pmatrix}\begin{pmatrix}1\\0\end{pmatrix}+\begin{pmatrix}1\\0\end{pmatrix}\begin{pmatrix}0\\1\end{pmatrix}=2\sqrt{2}(\downarrow\uparrow+\uparrow\downarrow)$. Using the above transformation of spin vectors one can get,

$$\mathbf{L_1}.\sigma|\chi_{1,1}>=2\sqrt{2}L_+{}^1\chi_{1,0}+2\sqrt{2}.0+2L_z^1\chi_{1,1} \tag{28}$$

$$\mathbf{L_1}.\sigma|\chi_{1,0}>=2\sqrt{2}L_+{}^1\chi_{1,-1}+2\sqrt{2}L_-{}^1\chi_{1,1}+L_z^1.0 \tag{29}$$

$$\mathbf{L_1}.\sigma|\chi_{1,-1}>=2\sqrt{2}L_+{}^1.0+2\sqrt{2}L_-{}^1\chi_{1,0}-2L_z^1\chi_{1,-1} \tag{30}$$

The spin average of the operator $\mathbf{L_1}.\sigma$ turns out to be

$$\begin{pmatrix}\chi_{11}&\chi_{10}&\chi_{1-1}\end{pmatrix}\begin{pmatrix}2\sqrt{2}L_+{}^1\chi_{1,0}+2\sqrt{2}.0+2L_z^1\chi_{1,1}\\ 2\sqrt{2}L_+{}^1\chi_{1,-1}+2\sqrt{2}L_-{}^1\chi_{1,1}+L_z^1.0\\ 2\sqrt{2}L_+{}^1.0+2\sqrt{2}L_-{}^1\chi_{1,0}-2L_z^1\chi_{1,-1}\end{pmatrix}=\begin{pmatrix}2L_z^1&0&0\\0&0&0\\0&0&-2L_z^1\end{pmatrix}.$$

Similarly the spin average for the $\mathbf{L_2}.\sigma$ tantamounts to
$\begin{pmatrix} 2L_z^2 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -2L_z^2 \end{pmatrix}$.
And finally for $(L_{12} + L_{21}).\sigma$
the spin average turns out to be $\begin{pmatrix} 2(L_z^{12} + L_z^{21}) & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -2(L_z^{12} + L_z^{21}) \end{pmatrix}$.

So combining all the contributions the diagonal elements of the spin orbit correction for He triplet P state in $J = L = M$ basis can be expressed as

$$\frac{1}{4c^2}[(\int\int \psi_{LL}{}^*(r_1{}^{-3}L_{1z} + r_2{}^{-3}L_{2z}) \times \times\psi_{LL}dv_1dv_2) - 3\int\int \psi_{LL}{}^* r_{12}{}^{-3}(L_{12z} + L_{21z})\psi_{LL}dv_1dv_2] \tag{31}$$

And similarly we can write the spin orbit contribution for all the operators.

5. CONNECTION BETWEEN THE SPIN ALGEBRA AND QUANTUM COMPUTING

In the early 1980s, Paul Benioff of Argonne National Laboratory and Richard Feynman of the California Institute of Technology began exploring the idea of using quantum-mechanical systems—such as individual atoms—as the building blocks of computation[10]. They demonstrated that, in principle, these tiny structures could function effectively as components in a quantum computer. Their work also introduced the concept of "quantum logic gates," proposing that computation could follow the fundamental rules of quantum mechanics.

To calculate spin-spin and spin-orbit interaction in Breit Hamiltonian (3) by linear algebra, we actually measure spin observables using state vector representation in quantum mechanics. On the classical (silicon based)computers information are stored by the bits 0 or 1. So for two particles the classical gates can store one of the four states at a time; 00, 01,10 or 11 whereas superposition principle allows quantum computers(atoms or subatomic particles) to store all four states simultaneously. This makes the quantum computers faster than classical ones. Bits in classical computers are equivalent to qubits in quantum computers. Quantum computers make use of the superposition principle which allows a system to be in 0 and 1 state simultaneously. For n q-bits there will be 2^n states or information. Quantum computers also exploit one more unique quantum property namely, quantum entanglement where a property of a particle can be linked to another regardless of the distance between them.

Qubits are atoms, ions and molecules. Suppose an electron is subjected to some electromagnetic field and spin of the electron is aligned with the field then it is said to be in the spin up state and in the opposite situation it will have a spin down state. The electron's spin can be changed by directing a pulse of energy to the particle by a laser beam/microwave. Each time the pulse is delivered, the electron spin state changes. If the half of the required energy is delivered to flip from one state to the other the electron will enter a superposition state and it will remain in that state until it is observed and measured.

General Quantum States If in a k-dimensional quantum system we have $|1>, |2>, ..., |k>$ as basis vectors the general state can be represented as $\alpha_1|1> + \alpha_2 > |2> + ... + \alpha|k>$ with $|\alpha_1|^2 + |\alpha_2|^2 + ... + |\alpha_k|^2 = 1$. 2^k dimensional system can be constructed as a tensor product of k quantum bits.

Unitary transforms: Linear transformations that preserve vector norm.

General Measurements:Let $|\psi_0>$, $|\psi_1>$ be two orthogonal one-qubit states, the $|\psi>= \alpha_0|\psi_0> + \alpha_1|\psi_1>$ Measuring $|\psi>$ gives $|\psi_i>$ with probability $|\alpha_i|^2$. This is equivalent to mapping $|\psi_0>$, $|\psi_1>$ to $|0>$ and $|1>$ then measuring. In section 3 we derived the matrix elements due to spin-spin and spin-orbit interactions for He (with spin half electrons) and we used the following basis states: ↑↑, ↓↑, ↑↓ and ↓↓. Or in other words the general spin state of a He atom can be written as $|S_{12}>= C_+ \uparrow\uparrow + C_- \downarrow\downarrow + C_0\frac{1}{\sqrt{2}}(\uparrow\downarrow + \downarrow\downarrow)$.

6. RESULTS AND DISCUSSIONS

In this paper using Naimark's extension formula we upgrade the spin-spin and spin-orbit operators in the extended Hilbert space and specifically calculate all the matrix elements connected to the spin-spin and spin-orbit operators in Breit's Hamiltonian for the triplet P-state of helium. In Section 4, we present our linear algebraic results pertaining to these corrections. Specifically, subsection 4.4 and 4.5 deal with the spin-spin and spin-orbit corrections respectively. In subsection 4.4 and 4.5 Eqs.(6-19) represent our results for spin averages for spin-spin interaction and Eqs.(20-30) represent the results for the spin averages for spin-orbit interactions respectively. Our final results in these two cases Eq.(19) and Eq.(30) exactly match with the previous results[5-7] obtained from conventional quantum mechanics.

7. CONCLUSIONS AND OUTLOOK

This algebra of spin systems underpins fundamental interactions in qunatum mechanics. In many realistic scenarios, spin operators are accessed only partially, leading to effective descriptions via POVMs. Naimark's extension theorem ensures that these can always be embedded into full projective descriptions on enlarged spaces. This provides a powerful conceptual and computational framework linking quantum measurements, operator theory, and spin algebra in multi-particle systems.

This work is a gentle but rigorous introduction to quantum computing with linear algebraic approach where qubits are state vectors and quantum gates are matrices. In this work we have been able to calculate the matrix elements for the spin dependent terms in the Breit Hamiltonian by spin algebra for He, the simplest many body system as an alternative to conventional quantum mechanics. It enables us to extend this linear algebraic method to multi-electron systems for developing quantum gate based on spin algebra and investigate quantum circuit design using spin qubits and compare the performance of spin-based qubits with traditional qubits in terms of algorithmic efficiency. One can use this spin algebra to simulate electron interactions in condensed matter physics problems. It can also help in exploring to predict material properties or simulate quantum many-body effects that are challenging for classical computers. It can be further utilized to develop spin-based error correction for small quantum systems. Two other directions it can be extended are (i) studying the role of spin liquids and topologically ordered phases in the context of quantum computing (ii) investigating potential for using topologically protected spin qubits for fault tolerance. In several occasions quantum spin models can be applied in a meaningful ways:

(1) Quantum spin models describe collection of qubits in information theory.

(2) It can serve as a toy model in theories related to quantum gravity.

(3) It can offer new insights in functional analysis(theory of operators) and representation theory(quantum groups)

This work can immediately be extended in two different directions: (1) Following tensor algebra spin averages can be calculated for other few-electron systems. (2) One can use these spin algebraic results and calculate the spin-spin and spin-orbit corrections on a quantum computer to compare the results with those obtained on a silicon based computers [12, 13].

The application of Naimark's Extension Theorem in computing matrix elements of spin-spin and spin-orbit operators reveals their deep connection to generalized measurement theory. These operators, which do not correspond to jointly measurable observables, can be interpreted as effective measurements arising from projective operations on a larger Hilbert space. This not only aids in computational simplification but also provides conceptual clarity regarding the role of ancilla systems, nonlocal correlations, and measurement-induced transformations in two-electron quantum systems.

The matrix elements arising from spin algebra, such as those in the Breit Hamiltonian, influence Quantum error corrections(QEC)[16] and fault-tolerant quantum computation by providing insight into the nature of errors (like spin flips or decoherence) and allowing for the design of tailored QEC codes that specifically address the types of errors induced by these spin interactions. It also helps to optimize the fault-tolerant gate construction by understanding how these interactions affect qubits during quantum gates. and enhances the understanding of the error thresholds and noise models to ensure that quantum computations are resilient against the types of errors these interactions could cause. By incorporating these matrix elements into the design of quantum error correction and fault-tolerant circuits, one can ensure that quantum computations remain accurate even in the presence of spin-dependent errors, improving the reliability of the quantum computing system.

The matrix elements obtained through the linear algebraic approach in this study have been previously calculated using conventional quantum mechanics methods [5-7, 11]. The author's prior work on relativistic corrections [12, 13], performed on a silicon-based classical computer, utilized quantum Monte Carlo simulations with path integrals. In this paper, the linear algebraic approach is adopted to make the calculations feasible on a quantum computer. Furthermore, simple circuits using quantum logic gates are proposed for computing the matrix elements. This approach opens the possibility for benchmarking results from both classical and quantum computers (future work), allowing for a direct comparison of their performance.

The application of *Naimark's Extension Theorem* in deriving their matrix elements opens up a window into the structure of quantum measurements in such composite systems. This study explores the spin algebra of two-electron systems, using tensor products . Our results align with conventional quantum mechanical approaches, providing a foundation for quantum logic gates, algorithms, and error corrections. These findings open the avenues for advancements in spin-based quantum systems, including new algorithms and simulations.

Declaration of interests: The sole author has no conflicts of interest to declare. There is no financial interest to report.

Data availability statement: No data in this publication is to be made available under the study-participant privacy protection clause.

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СПІНОВА АЛГЕБРА ТА РОЗШИРЕННЯ НАЙМАРКА: НАВЧАЛЬНИЙ ПІДХІД ІЗ ПРИКЛАДАМИ

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Під час аналізу двоелектронних систем до взаємодій, що нас цікавлять, часто належать спін-спіновий оператор $\vec{S}_1 \cdot \vec{S}_2$ та спін-орбітальний оператор $\vec{L} \cdot \vec{S}$. Коли ці оператори діють на заплутані або нерозрізнені частинки, їх вимірювання та фізична інтерпретація можуть виходити за межі стандартної проективної структури. Цей посібник знайомить з алгебраїчною структурою спінових взаємодій у двох електронних квантових системах та встановлює її концептуальний та математичний зв'язок з *Теоремою розширення Наймарка*. На основі явних прикладів для двоелектронних систем ми демонструємо, як виникають спінові оператори у редукованих просторах Гільберта, і як *Теорема розширення Наймарка* забезпечує формальну основу для їх поширення на проективні вимірювання у розширених просторах. Застосування *Теореми розширення Наймарка* при виведенні їх матричних елементів відкриває вікно у структуру квантових вимірювань у таких складних системах.

Ключові слова: *розширення Наймарка; Гільбертів простір; алгебра Лі; гамільтоніан Брейта; квантові обчислення*