Quantum Information Processing with Posner Molecules - A Conceptual Framework

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Contents

1   About

This document provides a conceptual framework for quantum information processing with nuclear spins in biological contexts, as proposed by Mattew Fisher [1]. Combined with ongoing experimental efforts, this framework presents a foundation for potential applications in therapeutics, synthetic biology, and quantum computing.

An introductory-level familiarity with the formalism and concepts of quantum mechanics is assumed in some sections (see [[2]] for a modern introduction). For convenience, a brief summary of the ideas in quantum information processing is included in Appendix A.

2 Overview: Nuclear Spins in Biology

Conventional wisdom says that biological contexts are not conducive to quantum information processing. Briefly, the argument is that biological systems, which operate near thermal equilibrium, only support quantum states with extremely short lifetimes (think 10^{-13} - 10^{-20} seconds) [3]. If true, then there may simply be insufficient time for biologically-relevant quantum information processing to occur.

A careful consideration of nuclear spin states (reviewed in Appendix B) may provide an exception to this argument. The spin states of certain atomic nuclei are naturally well-isolated from their environment, providing non-equilibrium quantum states with lifetimes measured in *seconds* [4], a fact is regularly exploited by the (related) fields of nuclear magnetic resonance (NMR) spectroscopy, MRI, and NMR-based quantum computing.

For biology to leverage nuclear spins for quantum information processing, at least the following must be true (more specific requirements can be found in [1] and [5]):

1. A molecule with long-lived nuclear spin states is naturally present in biological contexts.

2. The nuclear spins must support non-trivial quantum states via some entangling mechanism.

3. The nuclear spins must actively inform the dynamics of the containing biological system, and vice versa.

The remainder of this document summarizes a theoretical model that predicts *all* of these requirements could be met. Requirement 1 is supported by a specific calcium phosphate molecule (see Long-lived Nuclear Spin States in Posner Molecules). Requirements 2 and 3 are met with a novel "quantum dynamical selection" (QDS) conjecture [6] that relates nuclear spin states to chemical reactions (see Entanglement Between Posner Molecules). Together, these form the scaffolding of testable hypotheses regarding biological quantum information processing with nuclear spins.

3   Long-lived Nuclear Spin States in Posner Molecules

The six phosphorous nuclear spins in $Ca_9(PO_4)_6$, also called a "Posner molecule", are hypothesized to be strongly isolated from the surrounding liquid environment. This section summarizes the theoretical basis for this hypothesis. Further details can be found in [1] and [7]

A biological Posner molecule is suspended in a warm aqueous solution. Why don't the myriad of interactions between the Posner molecule and the surrounding solution scramble (decohere) the nuclear spins? The following subsections answer this question by considering both rotational dynamics and magnetic interactions. Note, these same arguments underpin well-established NMR-based technologies, and are reproduced here for Posner molecules for completeness.

3.1   Protection from Rotational Dynamics

A Posner molecule performs roughly one trillion rotations per second in biological contexts. At this rate, the nuclear spins constitute only a tiny fraction of the overall angular momentum of a Posner molecule. The solution, when approximated as a classical fluid, is continuously "measuring" this angular momentum via its interactions with the Posner molecules. However, the precision on these measurements is insufficient to distinguish between different nuclear spin states. This indistinguishability implies that the nuclear spins should not entangle with the solution via these rotational dynamics. [1]

3.2   Protection from Magnetic Interactions

Each spin $\frac{1}{2}$ phosphorous nucleus has as magnetic dipole moment [1]. This implies it interacts with any magnetic fields present near the nucleus, which could originate from other nuclei / electrons within the molecule, or from magnetic dipoles (e.g. protons) in the surrounding fluid.

3.2.1   Coupling Between Phosphorous Nuclei

Interactions between the nuclear spins within a single Posner molecule are predicted to occur. However, these do not themselves provide a decoher-

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[1]: Crucially, spin $\frac{1}{2}$ nuclei do not couple to electric fields, which would otherwise rapidly decohere the state. Phosphorous and hydrogen contain the only two naturally-occurring spin $\frac{1}{2}$ nuclei in biology, but phosphorous is generally more protected.

ence pathway, which requires interactions with the external environment. Therefore, these interactions will be ignored for the present purposes.

3.2.2 Coupling Between Phosphorous Nuclei and Nearby Electrons

The electrons in a Posner molecule each have strong magnetic dipole moments, relative to the nuclear magnetic moment. These electron magnetic dipoles can couple both to a phosphorous nucleus and an external magnetic dipole, which provides a decoherence pathway. This is mitigated in the case of a Posner molecule, since each electron is generally in a pair with anti-aligned spins, which have no overall magnetic dipole moment.

3.2.3 Coupling Between Phosphorous Nuclei and External Magnetic Dipoles

Classical external magnetic fields can affect nuclear spin states by causing them to precess. In biological settings, such magnetic fields could originate from a nearby magnetic dipole in the solution (e.g. a hydrogen ion), or, for example, the strong static magnet of an MRI device.

Posner molecules in warm solutions are rapidly rotating relative to external magnetic dipole sources. Due to this motion, phosphorous nuclei in a Posner molecule experience an average field close to zero [1], which minimizes the field's effect on the spins. Interestingly, the protection due to this "motional narrowing" effect is predicted to positively correlate with the tumbling rate and, therefore, temperature.

Additionally, the nuclear spin states of interest (defined later as the "pseudospin sectors") have small or zero overall magnetic dipole moments. This fact also reduces their susceptibility to external magnetic fields.

3.3 Coherence Time Estimates

Given these considerations, the phosphorous nuclear spins in a Posner molecule are expected to be strongly isolated from the surrounding environment. Theoretical approximations assume that coupling between phosphorous nuclei and external magnetic dipoles (e.g. protons) is the dominant decoherence pathway. In section III.E.3 of [7], the timescale for depolarizing noise (T_1) was estimated to be *3 weeks* due to the coupling between phosphorous spins and an external proton. The dynamics of the molecule in a liquid imply that

5

dephasing noise acts on a similar timescale (i.e. $T_1 \approx T_2$).

Overall, these estimates suggest that quantum spin states within Posner molecules can be maintained for biologically-relevant timescales. Experiments (e.g. via NMR spectroscopy) to validate this prediction are underway.

4 Entanglement Between Posner Molecules

4.1 About

The nuclear spins of distinct Posner molecules are hypothesized to become entangled via chemical binding dynamics. This is a direct prediction of the QDS conjecture [6], which is relevant to Posner molecules due to their hypothesized three-fold rotational symmetry and long-lived nuclear spin states.

The following sections describe the theoretical model behind QDS, and apply it to the case of pairwise binding of Posner molecules.

4.2 Rotational Symmetry of Posner Molecules

A one likely configuration of the atoms in a Posner molecule exhibits 3-fold rotational symmetry [7] Following [6], the electrons in a Posner molecule are assumed to transform trivially under a $\frac{1}{3}$ rotation. Therefore, only the nuclear component is considered for the remainder of this document.

Let $\hat{C}_3$ represent the quantum operator which performs a $\frac{1}{3}$ rotation of the nuclei in a Posner molecule around the symmetry axis. Perfect 3-fold symmetry implies

$$\hat{C}_3 \psi = \psi. \tag{1}$$

That is, the wavefunction remains unchanged [2] after the rotation. Without loss of generality, ψ can be expanded to expose the spin and orbital degrees of freedom of the nucleus [3]:

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[2] If this rotation constituted an even cyclic permutation of identical Fermions (here, the phosphorous nuclei), then $\hat{C}_{even} |\Psi\rangle = -|\Psi\rangle$. However, for Posner molecules the permutation is odd, which implies no overall phase.

[3]: The meaning of indices τ and l is covered in the two subsequent sections.

$$\psi = \sum_{\tau,l} \psi_{spin}^{(\tau)} \psi_{orbital}^{(l)}. \tag{2}$$

$\hat{C}_3$ can be analyzed on the spin and orbital wavefunctions separately, via the following decomposition:

$$\hat{C}_3 = \hat{C}_3^{spin} \otimes \hat{C}_3^{orbital} \tag{3}$$

The following subsections analyze the rotational symmetry constraint embodied by equation 1 to find that *the spin and orbital degrees of freedom must be entangled.*

4.3 Cyclic Permutations of Phosphorous Spins

In a 3-fold symmetric Posner molecule, $\hat{C}_3^{spin}$ is a cyclic permutation of the phosphorous nuclear spin states [4]. The symmetry constraint drives focus on the eigenstates of $\hat{C}_3^{spin}$, which are invariant under cyclic permutation. Given that $(\hat{C}_3^{spin})^3 = \hat{I}$, we can deduce that the possible eigenvalues are the cube-roots of unity. Thus,

$$\hat{C}_3^{spin} \psi_{spin}^{(\tau)} = \omega^\tau \psi_{spin}^{(\tau)}, \tag{4}$$

where $\omega = e^{\frac{2\pi i}{3}}$, $\tau \in \{0, \pm 1\}$, and $\psi_{spin}^{(\tau)}$ [5] denotes any vector in the eigenspace associated with eigenvalue ω^τ.

τ is called the "pseudospin", and it labels how states in the three "pseudospin sectors" (eigenspaces) accumulate phase under the permutation $\hat{C}_3^{spin}$. The nuclear spin states in these sectors are enumerated in Tables I-IV of [5] and visualized in Figure 6 of [7]

The $2^6 = 64$ orthogonal eigenvectors of $\hat{C}_3^{spin}$ span the entire Hilbert space of the 6 phosphorous nuclear spins in a Posner molecule. Ignoring normalization, any arbitrary spin state for these nuclei can therefore be written as a linear combination [6] of vectors from each eigenspace:

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[4]The other nuclei in a Posner (oxygen and calcium) have nuclear spins of 0, so we ignore their states in this section.

[5]: The superscript (τ) in $\psi_{spin}^{(\tau)}$ denotes an index, not an exponent.

[6]: The uniqueness of this decomposition is not claimed here, nor is it leveraged in the logic that follows.

$$\psi_{spin} = \sum_{\tau} \psi_{spin}^{(\tau)}$$

4.4 Orbital Rotations of Phosphorous Spins

$\hat{C}_3^{orbital}$ represents a $\frac{1}{3}$ rotation of the positions of all nuclei in a Posner molecule around the symmetry axis. Define the operator $\hat{L}$ as a measurement of the angular momentum along the axis of symmetry. A rotation of angle ϕ is then represented by the unitary operator $\hat{R}(\phi) = e^{-i\phi\hat{L}}$ ($\hbar = 1$). So,

$$\hat{C}_3^{orbital} = \hat{R}(\frac{2\pi}{3}) = e^{-i\frac{2\pi}{3}\hat{L}} = \omega^{-\hat{L}}$$

where, again, $\omega = e^{\frac{2\pi i}{3}}$ is the cube-root of unity.

Now consider rotating the eigenstates of $\hat{L}$, denoted $\psi_{orbital}^{(l)}$:

$$\hat{C}_3^{orbital}\psi_{orbital}^{(l)} = \omega^{-\hat{L}}\psi_{orbital}^{(l)} = \omega^{-l}\psi_{orbital}^{(l)}. \qquad (5)$$

Thus, by definition, $\hat{C}_3^{orbital}$ imparts a phase of ω^{-l} to the angular momentum eigenstate with eigenvalue l.

4.5 Entanglement Between Pseudospin and Orbital Momentum

Combining equations 1, 2, 3, 4, 5, we find a relation between the phases found in the previous two sections:

$$
\begin{aligned}
\hat{C}_3\psi &= \hat{C}_3 \sum_{\tau,l} \psi_{spin}^{(\tau)}\psi_{orbital}^{(l)} \\
&= \sum_{\tau,l} \hat{C}_3^{spin}\psi_{spin}^{(\tau)}\hat{C}_3^{orbital}\psi_{orbital}^{(l)} \\
&= \sum_{\tau,l} \omega^{\tau}\psi_{spin}^{(\tau)}\omega^{-l}\psi_{orbital}^{(l)} \\
&= \sum_{\tau,l} \psi_{spin}^{(\tau)}\psi_{orbital}^{(l)} \\
&= \psi
\end{aligned}
$$

Thus, the rotational symmetry constrains the phase accumulated by each term, namely $\omega^{\tau}\omega^{-l} = 1$. This relates the values of τ and l:

$$\omega^{\tau}\omega^{-l} = \omega^{\tau-l} = e^{i\frac{2\pi}{3}(\tau-l)} = 1$$
$$\tau - l = 3\mathbb{Z}$$
$$l = \tau - 3\mathbb{Z}$$

where $\mathbb{Z}$ is the set of integers. The spin and orbital components of the nuclear wavefunction are therefore *entangled* [7]:

$$\psi = \sum_{\tau}\sum_{l\in\tau-3\mathbb{Z}} \psi_{spin}^{(\tau)}\psi_{orbital}^{(l)} \tag{6}$$

For example, if $|l| \approx 1000$, the pseudospin sectors could have the following angular momenta l [8]:

$\tau = +1$	$\tau = 0$	$\tau = -1$
...	...	...
999	1000	1001
1002	1003	1004
1005	1006	1007
...	...	...

4.6 Pseudospin Entanglement and Pairwise Posner Binding

In certain situations, the entanglement between pseudospin and orbital momentum becomes relevant to chemical dynamics [6]. One such case is when two Posner molecules (say A and B) attempt to chemically bind. During a pairwise binding, the two Posner symmetry axes are hypothesized to be anti-aligned (a claim supported by electronic structure simulations) [7] This implies that the relative angular momenta of the two chemically bound Posner molecules is constrained [9] by:

$$l_A = -l_B$$

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[7]: The entanglement in this expression is manifest by the values for l depending on the value of τ, which prevents any decomposition of the form $\psi = \psi_{spin} \otimes \psi_{orbital}$.

[8]: The corresponding negative values are equally likely, but not shown here.

[9]: Another way to imagine this constraint is that bound molecules are not slipping against each other.

Given the contents of the previous subsection, this constraint imposes a related constraint on the pseudospins:

$$\tau_A = -\tau_B \tag{7}$$

If the nuclear spin wavefunction for each molecule is represented as a superposition of states in each pseudospin sector, like

$$|\Psi\rangle = \sum_\tau \alpha_\tau |\tau\rangle ,$$

then the joint state of the bound [10] molecules is *entangled*:

$$|\Psi_{AB}\rangle_{bound} = \alpha_{0,0} |0\rangle_A |0\rangle_B + \alpha_{-1,+1} |-1\rangle_A |+1\rangle_B + \alpha_{+1,-1} |+1\rangle_A |-1\rangle_B$$

This state may persist after the Posner molecules unbind, providing a potential mechanism for distributing entanglement throughout a biological system. This pseudospin entanglement structure could furthermore modulate the probabilities of pairwise binding events within a set of Posner molecules, via a reciprocal argument to the one above. Since bound Posner molecules are predicted to be more vulnerable to hydrolyzation, which releases their calcium ions to the local environment, there is a hypothetical link between the pseudospin entanglement structure and calcium signaling. [1]

5 Hypothetical Mechanism for Lithium Isotope Effects

Simulations show it is energetically favorable for two Li^+ ions to take the place of the Ca^{2+} ion in the center of a Posner molecule [7] If this happens, the non-zero spins of the two Li nuclei will couple to the phosphorous spins, unlike the zero-spin Ca nucleus they replaced. Critically, this new dynamic would be sensitive to whether ^7Li (common) or ^6Li (rare) is involved, since these two stable isotopes have different nuclear spins. The difference is manifest in the decoherence times in water, which are 10 seconds for ^7Li and 5 *minutes* for ^6Li [8]. In this case, a single neutron makes a large difference!

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[10]: Here it is assumed that whether or not the two molecules bind constitutes a projective measurement of the quantum state of the pseudospins. Accordingly, the failure of two nearby Posner molecules to bind projects the pseudospins into a different entangled state.

The exact effect of the Li isotopes on Posner spin states is ongoing research. One reasonable hypothesis is that the coherence time [11] of the spins in a Posner is differentially affected by the isotope of Li present. This could partially account for the differential Lithium isotope effects observed in biological systems [1].

6 Prospects for Information Processing with Posner Molecules

The following is an inexhaustive list of open questions regarding the information processing capacity of Posner molecules:

1. What kinds of entangled states are supported by the pseudospins in a large [12] network of Posner molecules?

2. Are the allowed transformations of pseudospin states sufficient for universal quantum computation?

3. Can a natural or synthetic system implement quantum computation with Posner molecules?

The following subsections briefly summarize ongoing research in these directions, including some unpublished / preliminary results.

6.1 Clifford-based Quantum Circuit Simulations

The pseudospin entanglement dynamics of a large set of symmetric Posner molecules can be approximately simulated via a quantum circuit model. In the ongoing work, three primary approximations are made:

1. The pseudospin is only a two state system (i.e. a qubit), not usual three-state system as defined above.

2. The Posner molecules only bind and unbind along a 1-dimensional chain.

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[11]: The coherence time of a system refers to the average time between events that scramble its quantum state. These events are usually from uncontrolled interactions with the external environment.

[12]: For present purposes, a network of 1000 or more Posner molecules is considered "large".

3. All unitary operations are Clifford operations [13].

Together, these approximations enable the simulation of a large [12] number of Posner molecules on classical computers. The preliminary results of these simulations include the following:

1. Given enough time, all pseudospins will align in a pure quantum state, independent of the initial state or its purity.

2. The time to achieve this steady-state scales quadratically with system size. This allows for the possibility that the steady-state is achieved within the Posner nuclei's coherence time.

3. On shorter timescales, non-trivial entangled states emerge. Further characterizing these states is ongoing research.

6.2 Universal Quantum Computing

A universal quantum computer is a system that supports enough control of a quantum state to compute any unitary transformation and therefore, any quantum algorithm. In [5], the universality of Posner-based quantum computation is analyzed in the context of measurement-based quantum computing. Given sufficient assumptions about state-preparation, control of Posner binding, and the ability to perform local measurements, the authors were able to construct a cluster state that fueled universal measurement-based quantum computing with Posner molecules.

Showing the universality of Posner-based quantum computation with fewer or different assumptions is ongoing research.

6.3 Reservoir Computing

Reservoir computing is a machine learning framework used for the efficient classification of multivariate time-series data. It consists of a non-linear dynamic system, the "reservoir", which is coupled to an input stream and an output classifier. By training *only* the output classifier, the overall system can reach meaningful levels of classification performance [9].

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[13]: The Clifford operations constitute a restricted gate set that admits efficient time-evolution on classical computers. There is no physical motivation for this approximation - it is solely required for the feasibility of simulation.

Quantum systems are particularly appealing reservoirs due to their exponentially large state space and the non-linearity induced by projective measurements. There have been several attempts to leverage quantum systems in reservoir computing frameworks [10], [11], [12], [13], [14]. Notably for present purposes, one group demonstrated simple functions can be learned on a small NMR-based quantum reservoir computer [13].

Whether a collection of Posner molecules can be leveraged as a quantum reservoir for machine learning is an open question. Crucially, a computational framework like this might avoid the requirement of precisely controlling the binding of Posner molecules, since the reservoir is assumed to be stochastic and largely uncontrolled.

7   Acknowledgments

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8   References

9   Appendix A: A Review of Quantum Information

9.1   The Qubit

The fundamental unit of quantum information is the "qubit", which can be physically embodied by any two-state degree of freedom that is strongly isolated from its environment. A measurement operation that distinguishes the two states is called a "readout". In the measurement basis, a qubit has the generic state:

$$|\Psi_1\rangle = \alpha_0 |0\rangle + \alpha_1 |1\rangle$$

where $\alpha_i \in \mathbb{C}$ are the complex "probability amplitudes" and the sum indicates a "quantum superposition". The states $|0\rangle$ and $|1\rangle$ are called "computational basis states" and correspond to the states of a classical bit.

9.2   Multiple Qubits

Qubits compose into larger systems like any other quantum states. A system of N qubits has the generic state:

$$|\Psi_N\rangle = \sum_{i=0}^{2^N-1} \alpha_i \, |i\rangle$$

This is an assignment of a probability amplitude to each of the 2^N computational basis states $|i\rangle \in \{|00...0\rangle, |00...1\rangle, ... |11...1\rangle\}$. Here, the binary representation of the multi-qubit basis state is a shorthand for the tensor product of individual qubit states. The notation makes the following three representations equivalent: $|0\rangle_A \otimes |1\rangle_B = |0\rangle_A |1\rangle_B = |01\rangle_{AB}$. The subscripts labeling the subsystems are often dropped when the context makes them obvious or unnecessary.

9.3   Entanglement

Entangled states are defined as states which do not admit a full factorization into the states of their constituent qubits. Consider two qubits A and B, each initially in an equal superposition state. Before interacting, their combined state is (ignoring amplitude normalization):

$$|\Psi_{initial}\rangle = |00\rangle_{AB} + |01\rangle_{AB} + |10\rangle_{AB} + |11\rangle_{AB} = (|0\rangle + |1\rangle)_A (|0\rangle + |1\rangle)_B$$

This state is easily *factored* into separate states for A and B. After an entangling interaction, the state could become:

$$|\Psi_{entangled}\rangle = |00\rangle_{AB} + |11\rangle_{AB}$$

which cannot be factored into a product of states for A and B.

In this sense, entangled states correspond to situations where *the whole is richer than the sum of its parts*.

9.4   Measurement

Just like any other quantum state, a "quantum measurement" of $|\Psi_N\rangle$ results in outcome $|i\rangle$ with probability $|\alpha_i|^2$. The state after a measurement is irreversibly *collapsed* to $|\Psi_N\rangle = |i\rangle$, i.e. all amplitudes are 0 except α_i, which has magnitude 1. This is called the "Born Rule", and is usually presented as an axiom of quantum theory.

Note, the Born Rule implies the global scaling and phase of the amplitudes is physically meaningless. This reduces the real degrees of freedom embodied in a state of N qubits to $2 * 2^N - 2 = 2^{N+1} - 2$, which is still $\mathcal{O}(2^N)$.

9.5 Quantum Computation

A quantum computation is a set of operations that transform a state of N qubits to for the purpose of information processing. These operations are constrained by the laws of quantum physics, so not all transformations of the $\mathcal{O}(2^N)$ amplitudes are allowed. Specifically, any non-measurement operation must transform the state reversibly. These reversible transformations are called "unitary transformations". Any quantum computation can be described by some sequence of unitary transformations and measurement operations.

9.6 Quantum Speedup

A quantum speedup is an algorithmic advantage enabled by a quantum computation (when compared to a classical computation). Though there is no scientific consensus on the exact theoretical reason for quantum speedups, several algorithms with practical speedups have been discovered and demonstrated on real quantum computers. As the performance of quantum hardware improves, we expect these algorithmic speedups to enable "quantum advantage", defined as a real-world problem being solved faster / cheaper / better by leveraging quantum (rather than purely classical) resources.

10 Appendix B: A Review of Quantum Spin

10.1 Spin is Intrinsic Angular Momentum

Like mass and charge, all fundamental particles have an *intrinsic* value called "spin". Spin measures the intrinsic angular momentum of a particle, which affects both its rotational dynamics and its magnetic interactions. Quantum theory predicts that spin values take a *finite discrete spectrum*, which is notably different from the continuous model of classical angular momentum. Additionally, quantum theory predicts that, at any given time, only one axis of a particle's spin state can be measured. The foundations of spin quantization are understood via representation theory, which is beyond the scope of this summary. See [15] for a thorough introduction.

10.2 Spin $\frac{1}{2}$ Particles as Qubits

Consider a "spin $\frac{1}{2}$" particle (e.g. an electron) with spin $\pm\frac{\hbar}{2}$ along some measurement axis. In this basis, a generic quantum state for the spin is

given by

$$|\Psi_{spin}\rangle = \alpha \, |-\frac{\hbar}{2}\rangle + \beta \, |+\frac{\hbar}{2}\rangle \, .$$

This is a state in a two-dimensional complex Hilbert space, also known as a *qubit*. We can simplify the notation by moving to natural units ($\hbar = 1$) and re-labeling the states to $|0\rangle$ and $|1\rangle$:

$$|\Psi_{spin}\rangle = \alpha \, |0\rangle + \beta \, |1\rangle \, .$$

Qubits are reviewed in Appendix A.

10.3   Nuclear Spins

The spin of an atomic nucleus is given by the sum of the spins of its constituent protons and neutrons, which are both spin $\frac{1}{2}$ particles. When the spins of the protons and neutrons in a nucleus balance, the total nuclear spin is 0. When the spins aren't balanced, nuclei can have a net spin with magnitude $\in \{\frac{1}{2}, 1, \frac{3}{2}, 2, \frac{5}{2}, ...\}$.

11   Appendix C: Pseudospin Sectors

This appendix augments the subsection Cyclic Permutations of Phosphorous Spins. Please read that first.

The hypothesized three-fold rotational symmetry of a Posner molecule allows a decomposition of phosphorous nuclei into two triangles, each transforming independently during rotations along the symmetry axis. Therefore, the pseudospin sectors can be understood by considering permutations within triangle separately.

This section provides examples of triangle states invariant under $\hat{C}_3^{spin}$. Pairwise products of these states generate the vectors in the pseudospin sectors of the entire Posner molecule. See Tables I - IV of [5] for a complete enumeration.

As a reminder, the $\hat{C}_3^{spin}$ operation is a cyclic permutation that relabels the spin states. Explicitly, $\hat{C}_3^{spin} |abc\rangle = |bca\rangle$, where $a, b, c \in \{0, 1\}$ denote the spin states of the three nuclei within either triangle of phosphorous atoms in the Posner molecule.

11.1 Triangle States with Zero Accumulated Phase

Some examples of (unnormalized) triangle spin states that accumulate 0 phase under $\hat{C}_3^{spin}$ include $|000\rangle$, $|111\rangle$, and

$$|W\rangle = |001\rangle + |010\rangle + |100\rangle$$

since cyclic permutations of any of these is an identity operation (i.e. the accumulated phase is 1).

11.2 Triangle States with Accumulated Phase of ω

An example of an (unnormalized) triangle spin state that provides a global phase of ω under $\hat{C}_3^{spin}$ is

$$|\omega\rangle = |001\rangle + \omega^2 |010\rangle + \omega |100\rangle$$

.
Applying $\hat{C}_3^{spin}$:

$$
\begin{aligned}
\hat{C}_3^{spin} |\omega\rangle &= \\
\hat{C}_3^{spin} \left(|001\rangle + \omega^2 |010\rangle + \omega |100\rangle \right) &= \\
|010\rangle + \omega^2 |100\rangle + \omega |001\rangle &= \\
\omega |001\rangle + |010\rangle + \omega^2 |100\rangle &= \\
\omega \left(|001\rangle + \omega^2 |010\rangle + \omega |100\rangle \right) &= \\
\omega |\omega\rangle
\end{aligned}
$$

11.3 Triangle States with Accumulated Phase of ω^2

Similar to $|\omega\rangle$ defined in the last section, there is

$$|\omega^2\rangle = |001\rangle + \omega |010\rangle + \omega^2 |100\rangle$$

which can be verified to satisfy $\hat{C}_3^{spin} |\omega^2\rangle = \omega^2 |\omega^2\rangle$

11.4 Examples of States in Each Pseudospin Sector

Pairwise products of the (normalized) triangle states defined in the last sections provide the states in each pseudospin sector.

$\tau = 0$ includes all products of $|000\rangle$, $|111\rangle$, and $|W\rangle$. For example, $|W\rangle \otimes |111\rangle$ is in the $\tau = 0$ sector. The overall phase is $\omega^0 = 1$ under $\hat{C}_3^{spin}$, as required.

$\tau = 1$ includes $|000\rangle \otimes |\omega\rangle$, with overall phase ω^1 under $\hat{C}_3^{spin}$, as required.

$\tau = -1$ includes $|W\rangle \otimes |\omega^2\rangle$, with overall phase ω^2 under $\hat{C}_3^{spin}$, as required.

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