

GEOMETRIC ALGEBRA:

Imaginary Numbers Are Real

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LECTURE 2

On spin & spinors:

The operators for the x , y & z components of the angular momentum of a spin 1/2 particle (in units of \hbar) are usually represented by one half the **Pauli matrices**:

$$\underline{\sigma}_1 \equiv \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \quad \underline{\sigma}_2 \equiv \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix} \quad \underline{\sigma}_3 \equiv \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$$

These are easily seen to anticommute & square to the identity, and hence correspond to orthonormal vectors in a *matrix representation* for $G(3)$.

The state of a spin is more commonly specified by a **spinor** (unit vector) $|\psi\rangle$ in a 2-D Hilbert space H over \mathbb{C} , in which case the expected components of the angular momentum are

$$\frac{1}{2} \langle \psi | \underline{\sigma}_k | \psi \rangle = \frac{1}{2} \text{tr}(\underline{\Psi} \underline{\sigma}_k) = \frac{1}{4} \text{tr}(\underline{\Psi} \underline{\sigma}_k + \underline{\sigma}_k \underline{\Psi}) = \frac{1}{2} \text{tr}((\underline{\Psi} \bullet \underline{\sigma}_k) \mathbf{1}) = \underline{\Psi} \bullet \underline{\sigma}_k$$

where $\underline{\Psi} \equiv |\psi\rangle\langle\psi|$, i.e. the inner product of Ψ , $\sigma_k \in G(3)$!

Since $\Psi \bullet \sigma_k$ is a scalar, Ψ itself must be the sum of a scalar & a vector, and the scalar part is $\langle \Psi \rangle_0 \equiv \frac{1}{2} \text{tr}(\underline{\Psi}) = \frac{1}{2} \langle \psi | \psi \rangle = \frac{1}{2}$. Using the fact that the angular momentum is quantized along its own axis to $1/2$, the vector part can be written as $\frac{1}{2} \mathbf{R} \sigma_3 \tilde{\mathbf{R}}$, i.e. as a rotation of σ_3 by some spinor $\mathbf{R} \in G^+(3)$. It follows that $\Psi = \mathbf{R}(\frac{1}{2}(1 + \sigma_3))\tilde{\mathbf{R}}$ or, using the correspondence between $G^+(3)$ and $SU(2)$ matrices:

$$\underline{\Psi} = \begin{bmatrix} a & -b^* \\ b & a^* \end{bmatrix} \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix} \begin{bmatrix} a^* & b^* \\ -b & a \end{bmatrix} = \begin{bmatrix} a \\ b \end{bmatrix} \begin{bmatrix} a^* & b^* \end{bmatrix} = \begin{bmatrix} |a|^2 & ab^* \\ ba^* & |b|^2 \end{bmatrix} = |\psi\rangle\langle\psi|$$

Thus we can identify $|\psi\rangle$ with $\psi \equiv \mathbf{R}E_+$, where $E_+ \equiv \frac{1}{2}(1 + \sigma_3)$ is an **idempotent** ($E_+^2 = E_+$). In fact, since the 2nd column of $SU(2)$ matrices is determined by the first, we can just use \mathbf{R} !

Another big advantage of representing states by sums of scalars & vectors is that this representation extends directly to *statistical ensembles* $\{\Psi\}$ of spin states, as follows:

$$\bar{\Psi} = \frac{1}{M} \sum_{i=1}^M \Psi_i = \frac{1}{2} + \frac{1}{2M} \sum_{i=1}^M \mathbf{R}_i \sigma_3 \tilde{\mathbf{R}}_i \xrightarrow{M \rightarrow \infty} \frac{1}{2} + \oint \mathbf{R} \sigma_3 \tilde{\mathbf{R}} dP(\mathbf{R})$$

We may write this (dropping the bar) as $\Psi = (1 + s)/2$, where $s \equiv \|s\| \leq 1$ is the ensemble's **polarization**. The “operator” $\bar{\Psi}$, called the **density operator**, yields the *ensemble average expectation value* of any observable \mathbf{A} via:

$$\overline{\langle \psi | \mathbf{A} | \psi \rangle} = M^{-1} \sum_{i=1}^M \langle \psi | \mathbf{A} | \psi \rangle = 2M^{-1} \sum_{i=1}^M \langle \mathbf{A} \Psi_i \rangle_0 = 2 \langle \mathbf{A} \bar{\Psi} \rangle_0$$

Spins from Space-Time (sic)



The spin vector s is the net angular momentum (in units of \hbar), which for a classical spinning particle of charge e leads to a magnetic moment of $s\mu_0 \equiv se/(2m)$ ($c = 1$), where μ_0 is the **Bohr magneton**. The spatial vector s corresponds to a *space-time bivector* $s = s\gamma_0$, where γ_0 defines its inertial frame. In a co-moving frame, this evolves according to the covariant form of Lorentz equation (**Lecture 3**) as $\dot{s} =$

$$2\mu_0(\mathbf{F} \bullet (s\gamma_0)) \wedge \gamma_0 = 2\mu_0((\mathbf{E} \bullet s + (\mathbf{1}\mathbf{B}) \bullet s)\gamma_0) \wedge \gamma_0 = 2\mu_0 s \times \mathbf{B},$$

where we have used the facts that γ_0 anticommutes with s , \mathbf{E} , \mathbf{B} and $\mathbf{1}$, while $\mathbf{E} \bullet s$ is a scalar but $(\mathbf{1}\mathbf{B}) \bullet s$ is a spatial vector. The lack of response to the electric field is a result of choosing a co-moving frame. Thus the magnetic moment of the electron, which is very nearly $2\mu_0$, can be explained by a simple *classical* model. Like the magnetic field itself, however, spin behaves under inversion like a spatial bivector $\mathbf{1}s$.

MULTIPARTICLE ALGEBRA

More than the Sum of Its Parts?

To model a system of N particles:

- ➔ Take as usual the direct sum of their states (vectors);
- ➔ Consider the corresponding *joint* Clifford algebra, i.e. $(G(1, 3))^N \approx G(N, 3N)$;
- ➔ This algebra has dimension 2^{4N} (*exponential* in $N!$).

Assuming there exists a *common* frame of reference, i.e. a natural choice of time-like γ_0^m in every particle space, then:

- ➔ The even subalgebras $G^+(1, 3)$ of different particle spaces *commute*, since for $1 \leq i, j \leq 3$ and $1 \leq k < l \leq N$

$$\sigma_k^m \sigma_l^n \leftrightarrow (\gamma_k^m \gamma_0^m)(\gamma_l^n \gamma_0^n) = (\gamma_l^n \gamma_0^n)(\gamma_k^m \gamma_0^m) \leftrightarrow \sigma_l^n \sigma_k^m$$

where the superscripts are particle indices.

- ➔ Thus one has an isomorphism with the **tensor product** of the corresponding 3-D Euclidean geometric algebras:

$$(G^+(1, 3))^N \approx (G(3))^{\otimes N};$$

- ➔ This algebra has dimension 2^{3N} (still *exponential!*).

PRODUCT OPERATORS

The usual nonrelativistic theory of N spin 1/2 particles relies entirely upon the algebra of $2^N \times 2^N$ matrices over \mathcal{C} , which has dimension only 2^{2N+1} . The extra degrees of freedom in the algebra $(G^+(1, 3))^N$ are due to the fact that it contains a different imaginary unit ι^m for every particle m .

These extra degrees of freedom can be removed can be removed by multiplication by the **correlator idempotent**:

$$\mathcal{C} \equiv \frac{1}{2}(1 - \iota^1 \iota^2) \frac{1}{2}(1 - \iota^1 \iota^3) \cdots \frac{1}{2}(1 - \iota^1 \iota^N)$$

This projects everything onto an “ideal” of the correct dimension, in which all these different imaginary units have been identified. In addition, since $\mathcal{C} = \mathcal{C}^2$ is easily seen to commute with everything in the algebra, multiplication by it is trivially a homomorphism onto this ideal (subalgebra).

Henceforth we shall drop the implicit factor of \mathcal{C} from all our expressions, and use the single imaginary unit

$$\iota \equiv \iota^1 \mathcal{C} = \dots = \iota^N \mathcal{C}.$$

Note the correlated product of the even subalgebras in each particle space, $(G^+(3))^{\otimes N} / \mathcal{C}$, is a subalgebra of dimension 2^{2N} (the same as that of the subspace of Hermitian matrices), which has *never* been recognized in the matrix algebra!

MULTIPARTICLE SPINORS

Just as in the one-particle case, multi-particle spinors (state vectors) $|\psi\rangle$ in the 2^N -D complex Hilbert space correspond to elements of a left-ideal obtained by multiplying through by an idempotent:

$$EC \equiv E_+^1 \dots E_+^N C \quad (E_{\pm}^m \equiv \frac{1}{2}(1 \pm \sigma_3^m)).$$

This ideal corresponds, as before, to matrices whose columns are all zero save for their left-most, and provides a carrier space for the products of all possible 3-D rotations.

Similarly, multiparticle density operators may now be written (omitting now the C) as

$$\Psi = \frac{1}{M} \sum_{i=1}^M \Psi_i = \frac{1}{M} \sum_{i=1}^M \psi_i \tilde{\psi}_i = \frac{1}{M} \sum_{i=1}^M \mathbf{R}_i \mathbf{E} \tilde{\mathbf{R}}_i,$$

where $\mathbf{R}_i \in (G^+(3))^{\otimes N} / \mathcal{C}$. Note however that \mathbf{R}_i may not be *factorizable* into one particle rotations $\mathbf{R}_i^1 \dots \mathbf{R}_i^N$, in which case the corresponding spinor $\psi_i = \mathbf{R}_i \mathbf{E}$ cannot be expressed as a product of one-particle spinors $\psi_i^1 \dots \psi_i^N$ and so is termed *entangled*. It may also happen that the individual terms in this sum can be factorized as $\mathbf{R}_i^m \mathbf{E}_+^m \tilde{\mathbf{R}}_i^m$, but the overall sum is *not* factorizable. In this case the density operator describes a correlated, but not an entangled, statistical ensemble.

THE BASICS OF QUANTUM INFORMATION PROCESSING

Binary information can be stored in an array of two-state quantum systems (e.g. spin 1/2) *relative to* a fixed **computational basis** of $H(2^N)$ (or ideal in $(G(3))^{\otimes N}/C$):

$$|0\rangle = \begin{bmatrix} 1 \\ 0 \end{bmatrix} \leftrightarrow |0\rangle\langle 0| = \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix} \leftrightarrow E_+ = \frac{1}{2}(1 + \sigma_3)$$

$$|1\rangle = \begin{bmatrix} 0 \\ 1 \end{bmatrix} \leftrightarrow |1\rangle\langle 1| = \begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix} \leftrightarrow E_- = \frac{1}{2}(1 - \sigma_3)$$

Each such **qubit** can be placed into a **coherent superposition** over these two basis states, which for $\alpha, \beta \in C$ can be written in the following equivalent ways:

$$\alpha|0\rangle + \beta|1\rangle = \begin{bmatrix} \alpha \\ \beta \end{bmatrix} \leftrightarrow$$

$$(\alpha|0\rangle + \beta|1\rangle)(\tilde{\alpha}\langle 0| + \tilde{\beta}\langle 1|) = \begin{bmatrix} |\alpha|^2 & \alpha\tilde{\beta} \\ \tilde{\alpha}\beta & |\beta|^2 \end{bmatrix} \leftrightarrow$$

$$(\alpha + \beta\sigma_1)E_+(\tilde{\alpha} + \tilde{\beta}\sigma_1) = \frac{1}{2}(1 + \Re(\tilde{\alpha}\beta)\sigma_1 + \Im(\tilde{\alpha}\beta)\sigma_2 + (|\alpha|^2 - |\beta|^2)\sigma_3)$$

A superposition over all qubits individually *expands* to a superposition over all integers in $\{0, \dots, 2^N - 1\}$, e.g.

$$|\Omega\rangle = 2^{N/2} \underbrace{(|0\rangle + |1\rangle) \dots \dots (|0\rangle + |1\rangle)}_N = 2^{N/2} \sum_{j=0}^{2^N-1} |j\rangle,$$

($|j\rangle \equiv |01\dots0\rangle$ is obtained by *binary* expansion of the integer j).

By the linearity of quantum mechanics, any unitary operation U on such a superposition operates on every term of its expansion *in parallel*, i.e.

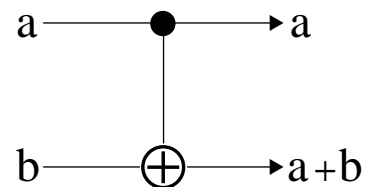
$$\underline{U}|\Omega\rangle = 2^{N/2} \sum_{j=0}^{2^N-1} \underline{U}|j\rangle$$

(in $(G^+(3))^{\otimes N}/\mathbb{C}$, U acts as $\underline{U}|\Omega\rangle\langle\Omega|\tilde{U}$, which is also linear). Moreover, there exists a polynomially-bounded basis for the unitary group $U(2^N)$ (i.e. one that is **unitarily universal**).

Example: All one-qubit operations, including those mapping one qubit states to superpositions, e.g. the **Hadamard gate**

$$\underline{R}_H|0\rangle = (|0\rangle + |1\rangle)/\sqrt{2} \quad \underline{R}_H|1\rangle = (|0\rangle - |1\rangle)/\sqrt{2},$$

together with the c-NOT (**controlled-NOT**) logic gate which computes the XOR of its inputs (see right). Note that this operates on bit b conditional on bit a .

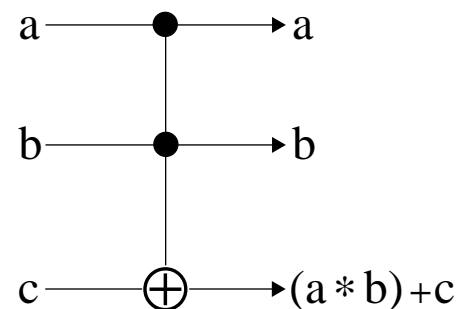


There exists a subgroup of $U(2^N)$ which:

- ➔ Maps single states $|j\rangle$ to single states.
- ➔ Admits a polynomially bounded basis for the symmetric group $S(2^N)$ (i.e. that is computationally **universal**).

This is nontrivial, since unitary operations are necessarily *reversible* (i.e. each output corresponds to a single input).

Example: The **Toffoli gate** has three input and three output bits. It copies the a & b bits, but takes the NOT of the c bit if the other two are both 1 (see right). Setting the c bit to 1 thus takes the NAND of the other two.



Some of the hardest and most interesting computational problems (e.g. NP-complete) are **decision problems**:

Given a boolean function $f: \{0, 1\}^N \longrightarrow \{0, 1\}^M$ **and an integer** $0 \leq j \leq 2^M - 1$, **decide if the set** $\{i \mid f(i) = j\}$ **has some global property (e.g. is nonempty, periodic, etc.).**

One might think such problems could be efficiently solved on a quantum computer by applying a unitary transformation U_f (which computes the function f) to a superposition,

$$\underline{U}_f(|\Omega\rangle|\mathbf{0}\rangle) = 2^{N/2} \sum_{i=0}^{2^N-1} |i\rangle|f(i)\rangle,$$

followed by measurement of the output qubit's state. But according to von Neumann's **measurement postulate**:

The result of a measurement on a quantum system in a superposition is a random term in the superposition, each with probability equal the modulus of its coefficient.

For $|\Omega\rangle|\mathbf{0}\rangle$, this implies the chance of observing a given $|j\rangle$ is

$$Pr(i | f(i) = j) = |\{i | f(i) = j\}| / 2^N,$$

which may be *exponentially* small. Even if it is not small, some properties of $\{i | f(i) = j\}$ (e.g. periodicity) can only be found by enumeration all or most of it.

There is a way around this: If one adjusts the *phases* of the terms of the input superposition appropriately, an additional transformation can be found that will *amplify* the magnitude of the coefficients associated with the solution(s), such that the probability of *finding* the solution upon making a measurement becomes appreciable. Because of an analogy with light diffraction, this is usually called **interference**.

Example: The Deutsch-Jozsa algorithm.

Suppose we are given a function $f: \{0, 1\} \rightarrow \{0, 1\}$, and ask:

➔ Is f a **constant** function, i.e.

$(|\{i | f(i) = 0\}| = 0) \text{ or } (|\{i | f(i) = 1\}| = 0)$, **or:**

➔ Is f a **balanced** function, i.e.

$|\{i | f(i) = 0\}| = |\{i | f(i) = 1\}|$ **??**

(two of the four possible functions $f: \{0, 1\} \rightarrow \{0, 1\}$ are constant, while the other two are balanced). This can be determined classically only by evaluating f on **both** inputs.

1) Starting with $|01\rangle \equiv |0\rangle|1\rangle$, apply the Hadamard gates:

$$|\psi_1\rangle \equiv (\underline{R}_H^1 \underline{R}_H^2) |01\rangle \equiv (\underline{R}_H |0\rangle)(\underline{R}_H |1\rangle) = \frac{1}{2}(|0\rangle + |1\rangle)(|0\rangle - |1\rangle)$$

2) Evaluate f via its unitary transformation U_f :

$$\begin{aligned} |\psi_2\rangle \equiv \underline{U}_f |\psi_1\rangle &= \frac{1}{2}(\underline{U}_f |0\rangle|0\rangle + \underline{U}_f |1\rangle|0\rangle - \underline{U}_f |0\rangle|1\rangle - \underline{U}_f |1\rangle|1\rangle) \\ &= \frac{1}{2}(|0\rangle|f(0)\rangle + |1\rangle|f(1)\rangle - |0\rangle|\bar{f}(0)\rangle - |1\rangle|\bar{f}(1)\rangle) \end{aligned}$$

where $\bar{f} = 1 - f$ is the **complement (or negation)** of f .

3) Using the fact that

$$|f(i)\rangle - |\bar{f}(i)\rangle = \begin{cases} |0\rangle - |1\rangle & \text{if } f(i) = 0 \\ |1\rangle - |0\rangle & \text{if } f(i) = 1 \end{cases} = (-1)^{f(i)}(|0\rangle - |1\rangle)$$

we can rewrite this as follows:

$$|\psi_2\rangle = \frac{1}{2}((-1)^{f(0)}|0\rangle + (-1)^{f(1)}|1\rangle)(|0\rangle - |1\rangle)$$

4) Now apply the same pair of Hadamard gates again:

$$\begin{aligned} |\psi_3\rangle &\equiv (\underline{R}_H^1 \underline{R}_H^2) |\psi_2\rangle \quad (\text{since } \underline{R}_H(|0\rangle - |1\rangle) = \sqrt{2}|1\rangle) \\ &= \frac{1}{2}((-1)^{f(0)}(|0\rangle + |1\rangle) + (-1)^{f(1)}(|0\rangle - |1\rangle))|1\rangle \end{aligned}$$

5) This in turn may be rewritten as

$$|\psi_3\rangle = \begin{cases} (-1)^{f(0)}|0\rangle|1\rangle & \text{if } f(0) = f(1) \\ (-1)^{f(0)}|1\rangle|1\rangle & \text{if } f(0) = \bar{f}(1) \end{cases}$$

showing the concentration of coherence via interference.

6) Thus measurement of the “input” (left-most) qubit gives $|0\rangle$ if f is *constant* and $|1\rangle$ if f is *balanced*.

The remarkable thing is that this took only a *single* evaluation of the function f . This algorithm was the first hint that quantum computers are more powerful than classical.

NB: A general quantum search algorithm is known which is quadratically faster than classical linear search, but *very* few quantum algorithms are known that are exponentially faster.

The Geometry Behind the Logic

The Hadamard Gate Revisited

Recall the action of the Hadamard gate on basis states:

$$\underline{R}_H|0\rangle = (|0\rangle + |1\rangle)/\sqrt{2} \quad \underline{R}_H|1\rangle = (|0\rangle - |1\rangle)/\sqrt{2} ,$$

The idempotents corresponding to the resulting states are:

$$\underline{R}_H \underline{E}_+ \tilde{\underline{R}}_H = \frac{1}{2} \begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix} \quad \Leftrightarrow \quad \underline{G}_+ \equiv (1 + \sigma_1)/2$$

$$\underline{R}_H \underline{E}_- \tilde{\underline{R}}_H = \frac{1}{2} \begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix} \quad \Leftrightarrow \quad \underline{G}_- \equiv (1 - \sigma_1)/2$$

We can also show that

$$\begin{aligned} \underline{R}_H(|0\rangle + \iota|1\rangle)/\sqrt{2} &= ((|0\rangle + |1\rangle) + \iota(|0\rangle - |1\rangle))/2 \\ &= ((1 + \iota)|0\rangle + (1 - \iota)|1\rangle)/2 \end{aligned}$$

which becomes $(|0\rangle - \iota|1\rangle)/\sqrt{2}$ on multiplying thru by the phase factor $(1 - \iota)/\sqrt{2}$. The corresponding idempotents are:

$$(|0\rangle \pm \iota|1\rangle)(\langle 0| \pm \iota\langle 1|) = \frac{1}{2} \begin{bmatrix} 1 & \mp \iota \\ \pm \iota & 1 \end{bmatrix} \quad \Leftrightarrow \quad \underline{F}_\pm \equiv (1 \pm \sigma_2)/2$$

Since $(\underline{R}_H)^2 = 1$ and maps $x \leftrightarrow z$ & $y \leftrightarrow -y$, it follows that \underline{R}_H is just a *rotation* by π about the axis $\underline{h} = (\sigma_1 + \sigma_3)/\sqrt{2}$!

Recall such rotations can be written in exponential form as

$$\exp(-\imath(\pi/2)\mathbf{h}) = -\imath\mathbf{h} \quad (\text{since } \mathbf{h}^2 = 1).$$

It may be observed that $(-\imath\mathbf{h})^2 = -1$, due to a geometrically irrelevant global phase (a **gauge** degree of freedom); the phase corrected Hadamard gate is

$$\mathbf{R}_H = \exp(\imath(\pi/2)(1 - \mathbf{h})) = \mathbf{h}; \quad \text{similarly,}$$

the NOT operation N is a rotation by π about σ_1 , i.e. $N = \sigma_1$.

The c-NOT Gate Revisited

Recall that the c-NOT gate takes the NOT of one qubit if the other is $|1\rangle$, e.g.

$$\begin{aligned} \underline{\mathcal{S}}^{2|1}|00\rangle &= |00\rangle & \underline{\mathcal{S}}^{2|1}|01\rangle &= |01\rangle \\ \underline{\mathcal{S}}^{2|1}|10\rangle &= |11\rangle & \underline{\mathcal{S}}^{2|1}|11\rangle &= |10\rangle \end{aligned}$$

Using the nilpotent **transition operators** $|0\rangle\langle 1|$ & $|1\rangle\langle 0|$, we can write this as

$$\begin{aligned} \underline{\mathcal{S}}^{2|1} &= |00\rangle\langle 00| + |01\rangle\langle 01| + |11\rangle\langle 10| + |10\rangle\langle 11| \\ &= |00\rangle\langle 00| + |01\rangle\langle 01| + \underline{\sigma}_1^2(|10\rangle\langle 10| + |11\rangle\langle 11|) \\ &= (|0\rangle\langle 0|)(|0\rangle\langle 0| + |1\rangle\langle 1|) + \underline{\sigma}_1^2(|1\rangle\langle 1|)(|0\rangle\langle 0| + |1\rangle\langle 1|) \\ &= |0\rangle\langle 0| \otimes \mathbf{1} + (|1\rangle\langle 1| \otimes \mathbf{1})\underline{\sigma}_1^2 \quad \leftrightarrow \quad \mathbf{E}_+^1 + \mathbf{E}_-^1 \underline{\sigma}_1^2 \end{aligned}$$

This has an interesting ideal-theoretic interpretation:

Rotate qubit 2 by π in the left-ideal defined by E_-^1 , but leave it alone in the complementary ideal defined by the annihilating idempotent E_+^1 .

Using a well-known formula for the exponential of any-thing times a commuting idempotent, this may be written as

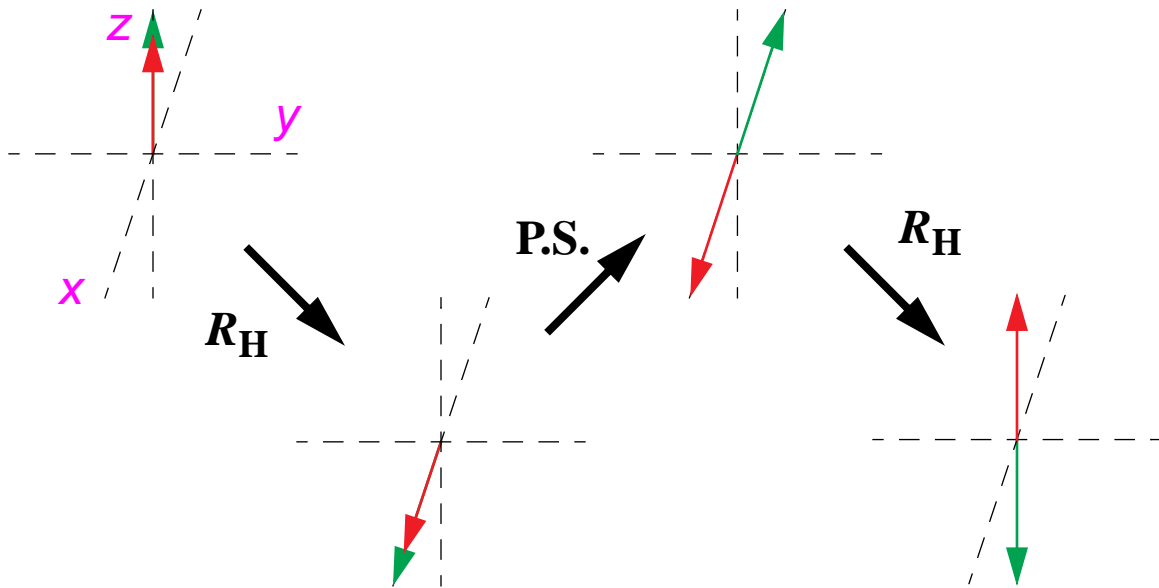
$$\begin{aligned} \exp(\imath(\pi/2)E_-^1(1 - \sigma_1^2)) &= (1 - E_-^1) + E_-^1 \exp(-\imath(\pi/2)(1 - \sigma_1^2)) \\ &= E_+^1 + E_-^1 \sigma_1^2 = 1 - 2E_-^1 G_-^2 . \end{aligned}$$

More generally, a **conditional rotation** is a rotation of a qubit in the left-ideal generated by the idempotents of the given states of one or more other qubits.

Noting that $\imath\sigma_3 E_{\pm} = \pm \imath E_{\pm}$ so that rotations about σ_3^1 in the ideal generated by G_-^2 are also conditional phase shifts, the form $1 - 2E_-^1 G_-^2$ makes it clear that $S^{2|1}$ can alternatively be viewed as a phase shift of the first qubit conditional on the second being along $-x$. We can therefore write $S^{2|1}$ as a phase shift conditional on both qubits being along $-z$, sandwiched between two Hadamards, as follows:

$$R_H^2 \exp(-\imath\pi E_-^1 E_-^2) R_H^2 = \exp(-\imath\pi E_-^1 R_H^2 E_-^2 R_H^2) = \exp(-\imath\pi E_-^1 G_-^2)$$

Using **green** & **red** arrows for the qubit projected onto the E_-^1 & E_+^1 ideals, this can be represented by vector diagrams as follows:



This is actually rather close to how $S^{2|1}$ is implemented in NMR spectroscopy, which also makes common use of such diagrams without recognizing their ideal-theoretic connection.

The Deutsch-Jozsa Algorithm Revisited

The initial superposition in the Deutsch-Jozsa algorithm is

$$|\psi_1\rangle\langle\psi_1| = G_+^1 G_-^2 = \frac{1}{4}(1 + \sigma_1^1 - \sigma_1^2 - \sigma_1^1 \sigma_1^2)$$

If $f(0) = f(1) = 0$, $U_f = 1$ and so the final Hadamards just transform this back to $E_+^1 E_-^2$, telling us it's constant.

Now suppose we have the function $f(0) = 0$, $f(1) = 1$. Then $U_f = S^{2|1}$, i.e. the output qubit is flipped from $|0\rangle$ to $|1\rangle$ when the input bit is $|1\rangle$. How does this act on the product operators in the initial state? To answer that question by geometric reasoning only, let us go into the ideals generated by G_-^2 and G_+^2 , where we find that

$$\sigma_1^1 \sigma_1^2 = \sigma_1^1 \sigma_1^2 (G_+^2 + G_-^2) = \sigma_1^1 G_+^2 - \sigma_1^1 G_-^2.$$

This shows that this state is that shown on the right, i.e. the two components of the first qubit point in opposite directions along x . We know that $S^{2|1} = 1 - 2E_-^1 G_-^2$ will rotate the green one by π about z to give us the state:

$$\sigma_1^1 G_+^2 + \sigma_1^1 G_-^2 = \sigma_1^1.$$

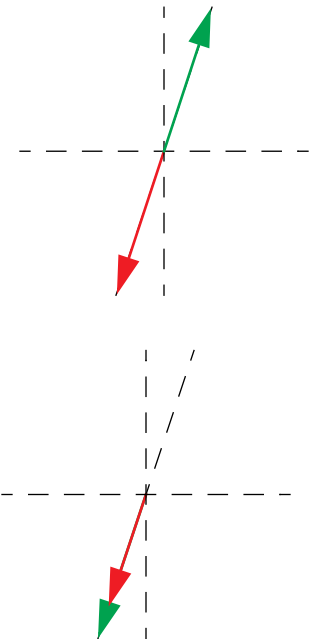
Thus the net effect of $S^{2|1}$ is to do a swap,

$$\sigma_1^1 \leftrightarrow \sigma_1^1 \sigma_1^2 ;$$

applied to $|\psi_1\rangle\langle\psi_1|$, it swaps the signs of these terms (while it commutes with & hence has no effect on σ_1^2), so we get:

$$S^{2|1} |\psi_1\rangle\langle\psi_1| S^{2|1} = \frac{1}{4} (1 - \sigma_1^1 - \sigma_1^2 + \sigma_1^1 \sigma_1^2) = G_-^1 G_-^2$$

The final Hadamards convert this to $E_-^1 E_-^2$ as expected.



CLOSING REMARKS

The Future of Quantum Computing

- 1) To date, computers have done more than theory has in enabling us to deal with *complexity* in the natural sciences (and elsewhere), because very simple local dynamics can model arbitrarily complex global behavior.
- 2) The situation in *multiparticle quantum systems* is similar: Simple (indeed linear) local dynamics can lead to very complex large-scale behavior, including the apparent nonlinearities of the classical world.
- 3) Quantum computers may yield only modest advantages in combinatorial problems, but they will certainly provide a powerful means of simulating *general* quantum systems.
- 4) Thus the advent of quantum computers will greatly extend the reach of *fundamental physics* to the complex systems found in *chemistry* and *molecular biology*.
- 5) Meanwhile, there is much to be learned about how simple quantum dynamics leads to classical complexity (even chaos), which is the subject of the theory of *decoherence*.
- 6) By computing with *homomorphic images* in Clifford algebras, this may even enable theorems to be “proved” by experiment (for CaF_2 , a dimension of $2^{10^{11}}$ has been reached).

THE BASICS OF NMR

A macroscopic quantum system:

Although the magnetic dipoles of near-by spins interact, the *rapid rotational diffusion* of the molecules in liquids average these interactions to zero. Hence to an excellent first-order approximation, spins in different molecules *do not interact*. It follows that if the state of the spins in the m -th molecule is $|\psi^m\rangle$, then density operator of an M molecule ensemble factorizes as follows:

$$\begin{aligned}\widehat{\Psi} &= \overline{|\psi^1\psi^2\dots\psi^M\rangle\langle\psi^1\psi^2\dots\psi^M|} \\ &= \overline{|\psi^1\rangle\langle\psi^1| \dots |\psi^M\rangle\langle\psi^M|} = \overline{|\psi^1\rangle\langle\psi^1|} \dots \overline{|\psi^M\rangle\langle\psi^M|} \\ &= \Psi^1\Psi^2\dots\Psi^M \approx \Psi^{\otimes M} \quad (\Psi \equiv M^{-1}\sum_m \overline{|\psi^m\rangle\langle\psi^m|})\end{aligned}$$

Thus the kinematics is identical to that of a single molecule!

The dynamics and observables are also identical, since:

$$\begin{aligned}e^{-it\sum_m \mathbf{H}^m} (\Psi^{\otimes M}) e^{it\sum_m \mathbf{H}^m} &= (e^{-it\mathbf{H}\Psi} e^{it\mathbf{H}})^{\otimes M} \\ \text{tr}\left(\Psi^{\otimes M} \sum_m \sigma_\alpha^m\right) &= M \text{tr}(\Psi \sigma_\alpha^m)\end{aligned}$$

The weak-coupling Hamiltonian:

The Hamiltonian of liquid-state NMR has the form:

$$\mathbf{H} = -\frac{1}{2}\sum_k \omega_0^k \sigma_3^k + \frac{\pi}{2}\sum_{k < l} J^{kl} (\sigma_1^k \sigma_1^l + \sigma_2^k \sigma_2^l + \sigma_3^k \sigma_3^l)$$

The first term is the Zeeman interaction (in rad/sec) with the external magnetic field (along z) as before; the second is the **scalar coupling** of pairs of spins across chemical bonds.

It follows from first-order perturbation theory that if $|\omega_0^k - \omega_0^l| \gg \pi J^{kl} \quad \forall k, l$ (weak coupling), the scalar coupling terms may be replaced by their secular parts $\pi J^{kl} \sigma_3^k \sigma_3^l$. Now since \mathbf{H} is diagonal, $\exp(-\imath t \mathbf{H})$ may be given in closed form.

Radio-frequency fields:

Given a strong RF-field on-resonance with the k -th spin,

$$\mathbf{H}_{\text{RF}} = \omega_1^k (\cos(\omega_0^k t) \sigma_1^k + \sin(\omega_0^k t) \sigma_2^k) = \omega_1^k \exp(\imath \omega_0^k t \sigma_3^k) \sigma_1^k$$

with $\omega_1^k \gg \pi |J^{kl}| \quad \forall l$, it follows from the Liouville-von Neumann equation that in a co-rotating frame

$$\Psi' = \exp(-\imath \omega_0^k t \sigma_3^k) \Psi \exp(\imath \omega_0^k t \sigma_3^k),$$

the (spin vector of) the spin rotates about the x' axis according to $\exp(-\imath \omega_1^k t \sigma_1^k)$. Henceforth, all our transformations will be referred to such a **rotating frame** (w/o primes).

In-Phase & Anti-phase Coherence

The effect of scalar coupling:

The (weak) scalar coupling propagator has the form:

$$\exp(-\imath\pi J^{12} t \sigma_3^1 \sigma_3^2 / 2) = \cos(\pi J^{12} t / 2) - \imath \sin(\pi J^{12} t / 2) \sigma_3^1 \sigma_3^2$$

Applied to a transverse state of e.g. spin 1, this yields:

$$\begin{aligned} \exp(-\imath 2\pi J^{12} t \sigma_3^1 \sigma_3^2 / 2) \sigma_1^1 \exp(\imath 2\pi J^{12} t \sigma_3^1 \sigma_3^2 / 2) \\ = \cos(\pi J^{12} t) \sigma_1^1 + \sin(\pi J^{12} t) \sigma_2^1 \sigma_3^2 \end{aligned}$$

This is a rotation between **in-phase** (σ_1^1) and **anti-phase** ($\sigma_2^1 \sigma_3^2$) coherence on spin 1.

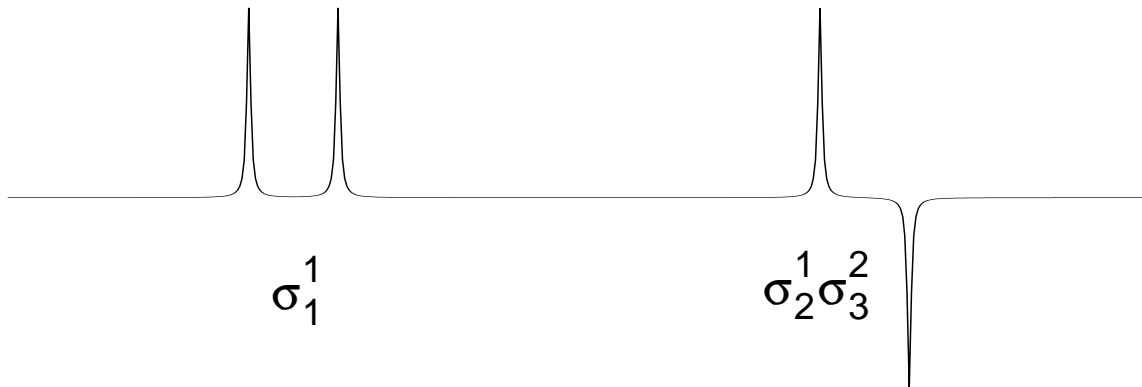
A classical interpretation is found on rotating to the z -axis, where the diagonal matrix elements in the σ_3 basis ($|0\rangle \equiv |\uparrow\rangle$, $|1\rangle \equiv |\downarrow\rangle$) are deviations from equal *populations*:

PO	$\langle 00 PO 00\rangle$	$\langle 10 PO 10\rangle$	$\langle 01 PO 01\rangle$	$\langle 11 PO 11\rangle$
σ_3^1	1	-1	1	-1
$\sigma_3^1 \sigma_3^2$	1	-1	-1	1

The anti-phase population *difference* between $|0\rangle$ & $|1\rangle$ states of spin 1 is inverted in the subensemble where spin 2 is down.

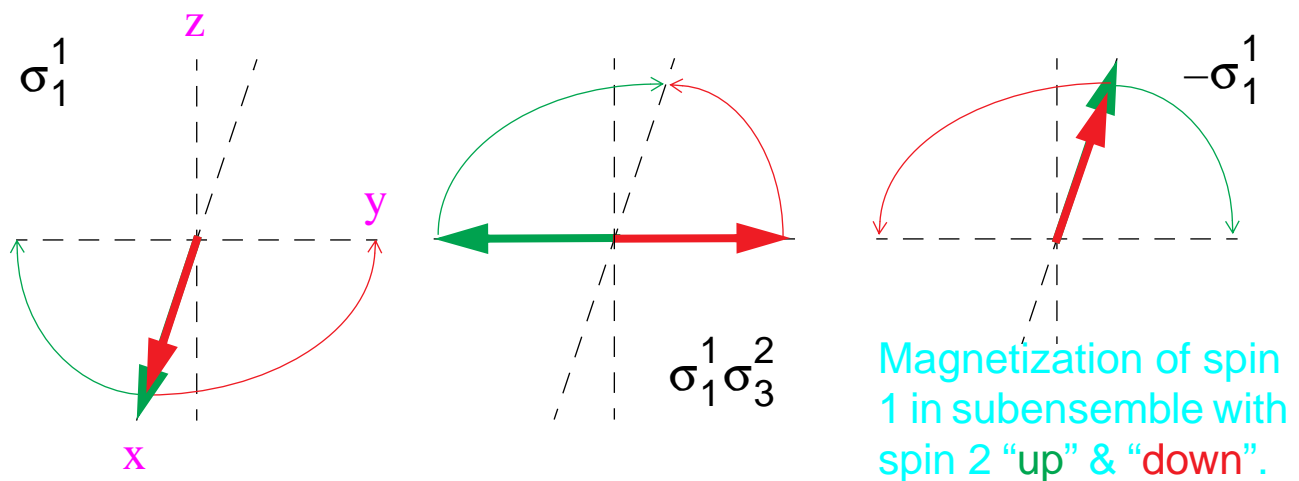
Spectra & vector diagrams:

Thus in- / anti-phase coherence corresponds to classical ensembles, characterized by these relative populations, which are *in transition* between spin 1 “up” & “down”. Moreover, spin 1’s magnetization (population difference) precesses at the rate $\omega_0^1/(2\pi) \pm J^{12}$ as spin 2 is “up” or “down”, resp. The spectrum (real part of the Fourier transform) is,



in which the anti-phase population inversion may be seen.

The rotation of σ_1^1 into $\sigma_2^1 \sigma_3^2$ may be visualized as follows:



The one-bit quantum logic gates:

The simplest logic gate is the NOT, which is a π -rotation about the x -axis combined with a phase shift,

$$\exp\left(i\frac{\pi}{2}(1 - \sigma_1^k)\right) = i(\cos(\pi/2) - i\sin(\pi/2)\sigma_1^k) = \sigma_1^k;$$

recalling that the density operators of the basis states of the k -th spin (with a totally mixed state everywhere else) are

$$(\mathbf{1} \otimes \dots \otimes |0\rangle\langle 0| \otimes \dots \otimes \mathbf{1}) = \frac{1}{2}(1 + \sigma_3^k) \equiv \mathbf{E}_+^k$$

$$(\mathbf{1} \otimes \dots \otimes |1\rangle\langle 1| \otimes \dots \otimes \mathbf{1}) = \frac{1}{2}(1 - \sigma_3^k) \equiv \mathbf{E}_-^k,$$

we can use the anticommutivity of σ_1^k & σ_3^k to show that this NOT gate maps the $|0\rangle$ state of the k -th spin to the $|1\rangle$ state:

$$\sigma_1^k \mathbf{E}_+^k \sigma_1^k = \sigma_1^k \frac{1}{2}(1 + \sigma_3^k) \sigma_1^k = (\sigma_1^k)^2 \frac{1}{2}(1 - \sigma_3^k) = \mathbf{E}_-^k$$

◆ Another important one-bit, but *nonboolean*, gate is the Hadamard transform HAD:

$$\exp\left(i\frac{\pi}{2}(1 - \sqrt{2}(\sigma_1^k + \sigma_3^k))\right) = \sqrt{2}(\sigma_1^k + \sigma_3^k),$$

which can be show to map $\sigma_1^k \leftrightarrow \sigma_3^k$ & $\sigma_2^k \leftrightarrow -\sigma_2^k$. It also maps $|0\rangle \leftrightarrow (|0\rangle + |1\rangle)/\sqrt{2}$ & $|1\rangle \leftrightarrow (|0\rangle - |1\rangle)/\sqrt{2}$, and so can be used to prepare a uniform superposition over all spins as above.

The multi-bit boolean logic gates:

Interesting computations require feedback, i.e. the state of one bit must influence what happens to another, but the usual AND & OR gates are *not* reversible (only one output!).

An important two-bit gate is the **controlled-NOT**:

$$\exp\left(i\frac{\pi}{2}(1 - \sigma_1^1)\mathbf{E}_-^2\right) = \sigma_1^1\mathbf{E}_-^2 + \mathbf{E}_+^2$$

This “c-NOT” is readily shown to flip the first spin in states where the second is down (just as we considered earlier), i.e.

$$|00\rangle \leftrightarrow |00\rangle \quad |10\rangle \leftrightarrow |10\rangle \quad |01\rangle \leftrightarrow |11\rangle \quad |11\rangle \leftrightarrow |01\rangle,$$

or more compactly: $|\delta^1\delta^2\rangle \leftrightarrow |(\delta^1 + \delta^2 \bmod 2)(\delta^2)\rangle$. Thus idempotents also describe the *conditionality* of operations.

Another obvious gate is the SWAP of two bits,

$$\exp\left(i\frac{\pi}{2}\Pi^{12}\right) = \Pi^{12} \equiv \frac{1}{2}(1 + \sigma_1^1\sigma_1^2 + \sigma_2^1\sigma_2^2 + \sigma_3^1\sigma_3^2);$$

Π^{12} is also called the **particle interchange operator**.

These can be extended to N bits; e.g., the **Toffoli gate** is:

$$\exp\left(i\frac{\pi}{2}(1 - \sigma_1^1)\mathbf{E}_-^2\mathbf{E}_-^3\right) = \sigma_1^1\mathbf{E}_-^2\mathbf{E}_-^3 + (1 - \mathbf{E}_-^2\mathbf{E}_-^3)$$

The TOF alone is *universal* for boolean logic; more generally, the c-NOT and one-bit rotations *generate* all of $SU(2^N)$.

NMR Implementations of Gates

Radio-frequency pulse sequences:

The NOT gate is easily implemented by a strong RF pulse, in phase with the x -axis, whose frequency range spans only the resonance of the target spin, and whose duration is sufficient to rotate it by π (note the global phase offset of \imath has no effect on the density operator).

The HAD gate is similarly obtained from the **pulse sequence** (written in left-to-right temporal order):

$$\left[\frac{\pi}{8}\sigma_2^k\right] \rightarrow \left[\frac{\pi}{2}\sigma_1^k\right] \rightarrow \left[-\frac{\pi}{8}\sigma_2^k\right] \Leftrightarrow \exp\left(\imath\frac{\pi}{8}\sigma_2^k\right)\exp\left(-\imath\frac{\pi}{2}\sigma_1^k\right)\exp\left(-\imath\frac{\pi}{8}\sigma_2^k\right)$$

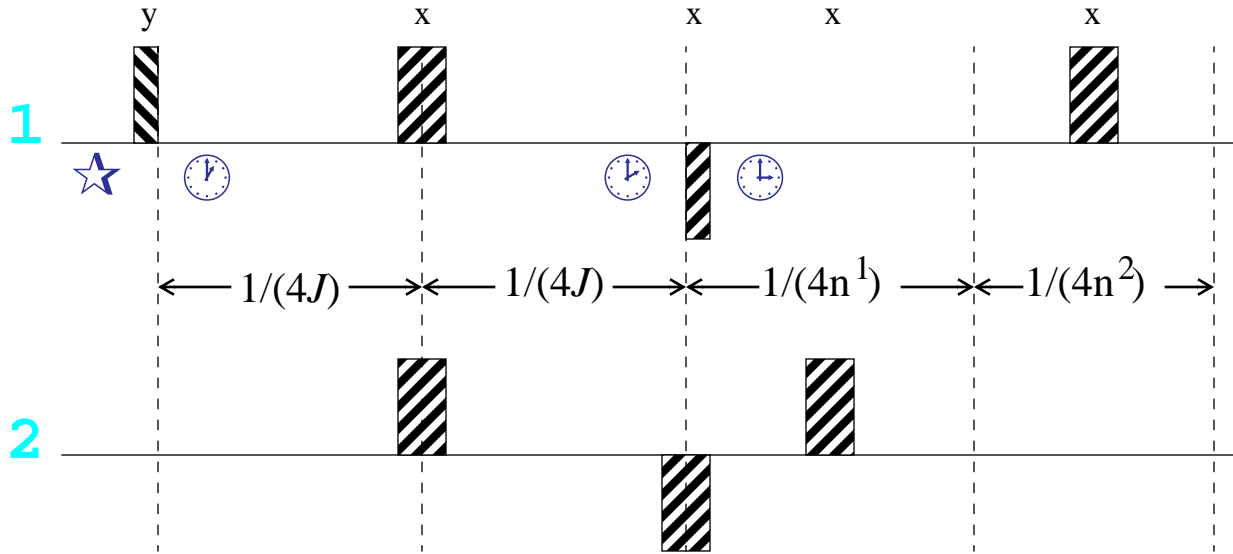
To implement the c-NOT gate, we proceed as follows:

$$\begin{aligned} \exp\left(\imath\frac{\pi}{2}(1 - \sigma_1^1)\mathbf{E}_-^2\right) &= \exp\left(-\imath\frac{\pi}{4}\sigma_2^1\right)\exp(\imath\pi\mathbf{E}_-^1\mathbf{E}_-^2)\exp\left(\imath\frac{\pi}{4}\sigma_2^1\right) \\ &= \exp\left(-\imath\frac{\pi}{4}\sigma_2^1\right)\exp\left(-\imath\frac{\pi}{4}(\sigma_3^1 + \sigma_3^2)\right)\exp\left(\imath\frac{\pi}{4}\sigma_3^1\sigma_3^2\right)\exp\left(\imath\frac{\pi}{4}\sigma_2^1\right)\sqrt{\imath} \\ &= \exp\left(-\imath\frac{\pi}{4}(\sigma_3^1 + \sigma_3^2)\right)\exp\left(-\imath\frac{\pi}{4}\sigma_1^1\right)\exp\left(\imath\frac{\pi}{4}\sigma_3^1\sigma_3^2\right)\exp\left(\imath\frac{\pi}{4}\sigma_2^1\right)\sqrt{\imath} \end{aligned}$$

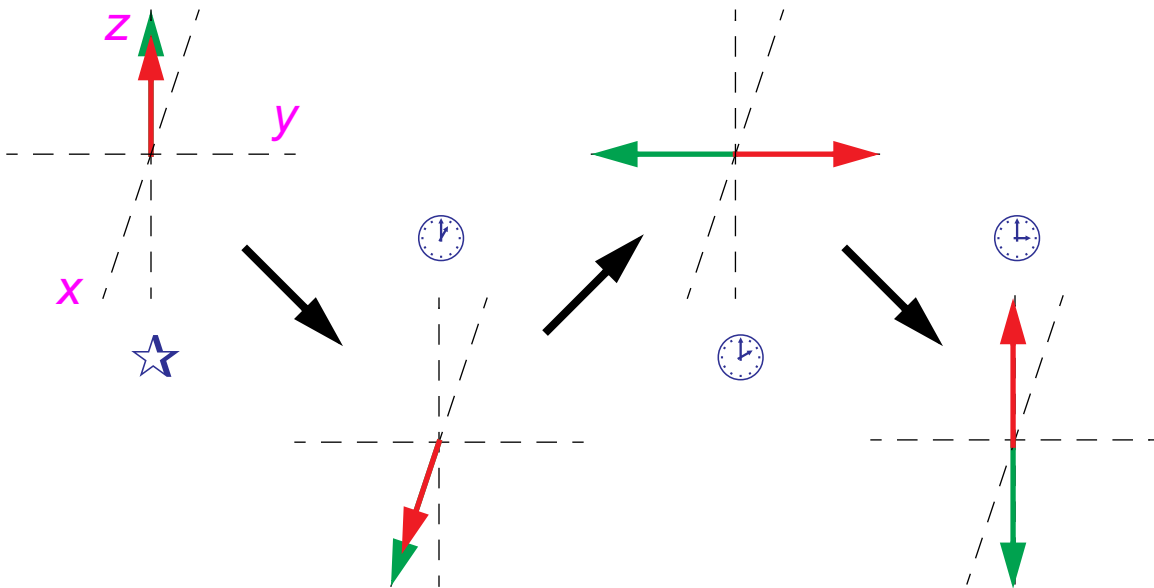
This is a $(\pi/2)$ -rotation about y , a weak coupling evolution for $1/(2J^{12})$, a $(\pi/2)$ -rotation about x , and a Zeeman evolution.

Vector diagram description:

◆ This pulse sequence may be depicted as follows:



In terms of Bloch diagrams, we have:



Caption: Here, **red** is magnetization of **1** spin in molecules where **2** spin is up, and **green** that of **1** spin where **2** down.

PSEUDO-PURE STATES

Starting from equilibrium:

Since $|2\pi J| \ll |\omega_0| \ll k_B T$, the **equilibrium state** of a homonuclear spin system (& its partition function $Q \approx 2^N$) is:

$$\Psi_{\text{eq}} = \frac{\exp(-\mathbf{H}_Z/k_B T)}{\text{tr}(\exp(-\mathbf{H}_Z/k_B T))} = \frac{\exp(-\sum_l \omega_0^l \sigma_3^l / 2k_B T)}{Q}$$

$$\approx (1 - \sum_l \omega_0^l \sigma_3^l / 2k_B T) 2^{-N} \approx \left(1 - \frac{\omega_0 \sum_i p_i |i\rangle \langle i|}{k_B T}\right) 2^{-N}$$

Here $|0101\dots 0\rangle$ is a binary expansion of $|i\rangle$, & $p_i = h(i) - N/2$ where $h(i)$ is the **Hadamard weight** (number of 1's) of i .

The problem with Ψ_{eq} is that logical operations performed on the spins at the *microscopic* level do not effect the same operations on their *macroscopic* polarizations; for two spins:

PO	$\langle 00 PO 00\rangle$	$\langle 10 PO 10\rangle$	$\langle 01 PO 01\rangle$	$\langle 11 PO 11\rangle$
$\rho_{\text{eq}} \quad \sigma_3^1 + \sigma_3^2$	1	0	0	-1
$\rho'_{\text{eq}} \quad \mathbf{E}_+^1 \sigma_3^2$	1	0	-1	0

Spin 1's polarization, i.e. the alternating row sum, goes to 0.

So we average yet more!

A **pseudo-pure state** is one whose density operator has exactly one nondegenerate eigenvalue, e.g.

$$\Psi_{\text{pp}} = \left(1 - \frac{\omega_0 p_0 |\mathbf{0}\rangle\langle\mathbf{0}|}{k_B T} \right) 2^{-N} \equiv (1 + \alpha |\mathbf{0}\rangle\langle\mathbf{0}|) 2^{-N}.$$

Note that the microscopic state $|\mathbf{0}\rangle = |00\dots 0\rangle$ is *canonically* associated with ρ_{pp} .

Because the identity component is unitarily *invariant*, the state $|i\rangle$ provides a *spinorial* representation of $\text{SU}(2^N)$:

$$\mathbf{U} \Psi_{\text{pp}} \tilde{\mathbf{U}} = (1 + \alpha (\mathbf{U}|\mathbf{0}\rangle)(\langle\mathbf{0}|\tilde{\mathbf{U}})) 2^{-N} \quad (\mathbf{U} \in \text{SU}(2^N))$$

Similarly, because the identity component does *not* contribute to the magnetization (population differences), the ensemble average expectation value of the observables is proportional to their ordinary *expectation values*:

$$\frac{1}{2} \text{tr}(\Psi_{\text{pp}} \sigma_1^k) = (\text{tr}(\sigma_1^k) + \alpha \text{tr}(\sigma_1^k |\mathbf{0}\rangle\langle\mathbf{0}|)) 2^{-N-1} = \frac{\alpha}{2^{N+1}} \langle\mathbf{0}|\sigma_1^k|\mathbf{0}\rangle$$

Since their eigenstructures differ, Ψ_{pp} must be prepared from Ψ_{eq} by a *nonunitary* process, e.g. by averaging the populations over all permutations of the states $|i\rangle\langle i|$ ($i > 0$) (more efficient methods exist, which rely upon magnetic gradients).