Zeroes of the Majorana polynomial and the quantum mechanics of spin

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(June 18, 2001)

A review of quantum mechanics through the example of two state systems is given. The Majorana representation of large spin is introduced and discussed in connection with spin dynamics in the semiclassical limit.

I. BRIEF REVIEW OF QUANTUM MECHANICS

We will give a brief review of quantum mechanics by way of an example of the most "non-classical" object: the two-state system (or its popular manifestation, the "qubit").

Quantum mechanics takes place in a vector space, spanned by basis vectors that represent the possible outcomes of an experiment. A physical example of such a two-state system might be a molecule that is either in its ground state or excited state, denoted respectively by $|m\rangle, |m^*\rangle$. In the present example, the two-dimensional vector space is spanned by two orthogonal basis vectors $\{|m\rangle, |m^*\rangle\}$ and an electric field could be used to make a measurement of which state the molecule is in [2] (if the excited state has a different electric dipole moment than the ground state).

The most general state of the molecule is, however, some linear combination of basis vectors

$$|\psi\rangle \equiv \alpha|m\rangle + \beta|m^*\rangle$$

Such states are in some sense a natural generalization to a classical bit, 0 or 1, representing the two possible states. If a measurement is performed with respect to these basis vectors, $|\alpha|^2 = \alpha\overline{\alpha}$ is the *probability* that the result will be "molecule in the ground state." Similarly $|\beta|^2$ is the probability that the molecule will be found in the excited state, and therefore, $|\alpha|^2 + |\beta|^2 = 1$. To express this property of probability, an inner product is introduced (along with the left side of "Dirac" notation: $\langle\psi|$):

$$\langle\psi|\psi\rangle = (\langle m|\overline{\alpha} + \langle m^*|\overline{\beta}) \times (\alpha|m\rangle + \beta|m^*\rangle) = |\alpha|^2 + |\beta|^2 = 1$$

State vectors representing physical systems must then have unit norm, i.e. $\langle\psi|\psi\rangle = 1$.

Observables physical quantities are represented by hermitian operators (we will give some examples later.) But also, hermitian operators are *generators* of unitary transformations, that is, transformations that preserve normalization. It is expected then, that time evolution must be generated by a particular hermitian operator. This special operator is called the hamiltonian denoted by H. Given the initial state of the system at t_0 (call it $|t_0\rangle$), the state of the system at time t is

$$|t\rangle = \exp -iH(t - t_0)|t_0\rangle \tag{1}$$

and the probabilities of all possible measurement outcomes will add up to one.

A. spin as a two-state system

We switch now to a different two-state system in which experiments are more easily visualized (and realized). Many elementary particles possess a small *intrinsic* angular momentum called "spin." The photon has spin, giving rise to familiar polarization effects. If the particles are charged, then spin will give rise to a magnetic moment. You can think of the magnet as aligned along the particle's spin axis.

Imagine taking a beam of these particles with their spin directions presumably pointing in random directions and passing the beam through an apparatus that the deflects the particle in proportion to their magnetic moment. Specifically, a magnetic field gradient along, say, the z-direction will exert a force on a magnet in the z-direction proportional to the z-component of the magnetic moment (as shown in figure 1). Classically, we would expect a continuous range of deflections in the z-direction but instead we observe only two possible "amounts of deflection." This is experimental evidence that we are dealing with a two-state system. Furthermore, if you are concerned that there is some bias present in the beam originally that skews the results, rotating the deflection apparatus would simply rotate the pattern.

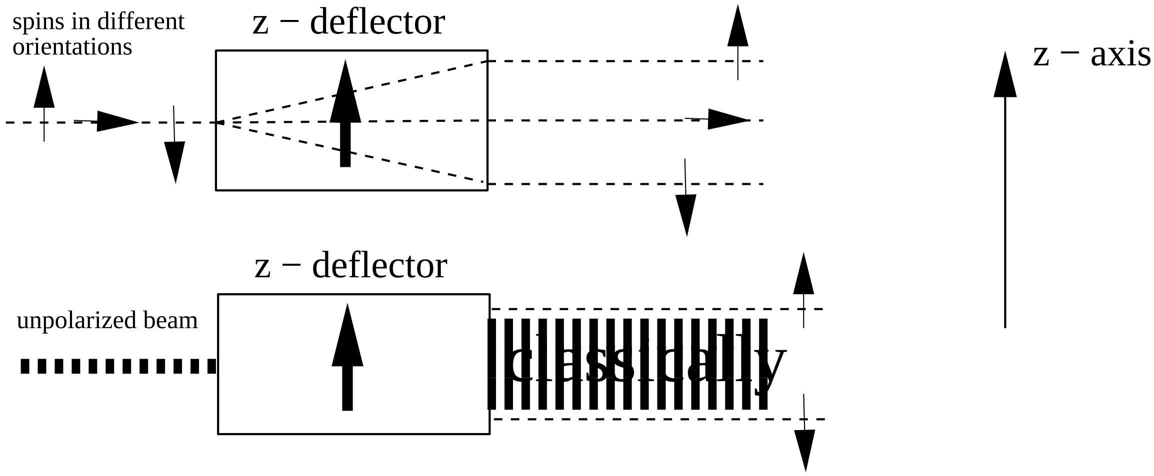

FIG. 1. Classical beam is deflected over a continuous distribution of displacements.

For the spin two-state system, we will denote the basis vectors by $|\uparrow\rangle$ $|\downarrow\rangle$. As mentioned before, in quantum mechanics observable quantities (e.g. momentum, energy, etc.) are represented by hermitian operators. It is possible to construct the operator corresponding to an observable quantity by first constructing *basis vectors* which represent the possible outcomes of the desired measurement of the observable quantity. The basis vectors then form a complete set of the eigenvectors of the operator we wish to construct.

Although this is a kind of trivial example—the operator s_z will corresponds to "spin angular momentum in the z-direction" or "z-polarization." Its eigenvectors are then the basis vectors that represent the possible outcomes of a measurement of spin in the z-direction. Thus it has as its eigenvectors $|\uparrow\rangle$ and $|\downarrow\rangle$ with eigenvalues $+\frac{1}{2}$ and $-\frac{1}{2}$ respectively, reflecting a positive or negative z-component of the spin angular momentum vector [3]. Writing $|\uparrow\rangle$, $|\downarrow\rangle$ as column vectors in the obvious way, a representation of s_z is:

$$|\uparrow\rangle_z \leftrightarrow \begin{pmatrix} 1 \\ 0 \end{pmatrix} \qquad |\downarrow\rangle_z \leftrightarrow \begin{pmatrix} 0 \\ 1 \end{pmatrix} \qquad s_z = \tfrac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

Once we have this operator, the average value of s_z in any state $|\psi\rangle$ (not necessarily an eigenstate) is obtained by "sandwiching" s_z and returns the (amount of "up") - (the amount of "down")

$$\langle\psi|s_z|\psi\rangle = |\alpha|^2 - |\beta|^2$$

Now imagine passing the beam that was deflected "up" through another deflector aligned along the z-axis. Presumably all spins in this beam are in the state $|\uparrow\rangle$; passing through the second detector seems to confirm this as they are simply deflected further "up". In this way beams of pure polarization may be created.

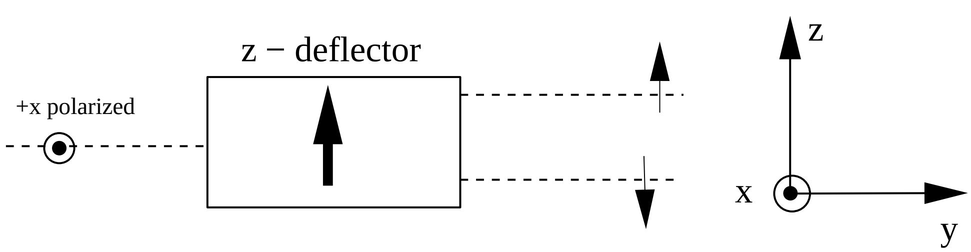

FIG. 2. Polarized in x is apparently equivalent to a superposition of "up" and "down" in z.

Suppose a pure beam of spins polarized in the x-direction is created and fed into the z-deflector (see figure 2). We would expect this beam to be undeflected; after all, it has no moment in the direction of the field gradient—*or does it?*. Surprisingly, the beam is split in two, half of the spins deflected up, half down. Polarized in x is apparently equivalent to a superposition of "up" and "down" in z:

$$|\uparrow\rangle_x = |\uparrow\rangle_z + |\downarrow\rangle_z \qquad |\downarrow\rangle_x = |\uparrow\rangle_z - |\downarrow\rangle_z$$

where the second equation follows from the orthogonality of $|\uparrow\rangle_x$ and $|\downarrow\rangle_x$ (we're ignoring normalization here). Since $|\uparrow\rangle_x, |\downarrow\rangle_x$ are the basis vectors for measurements of x-polarization, they are, by definition, the eigenstates of s_x with eigenvalues $\pm\frac{1}{2}$ and therefore,

$$s_x = \frac{1}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

Already, two of our "observables" s_z and s_x don't commute; this turns out to be a statement of the impossibility of preparing a state with well defined x *and* z components of polarization.

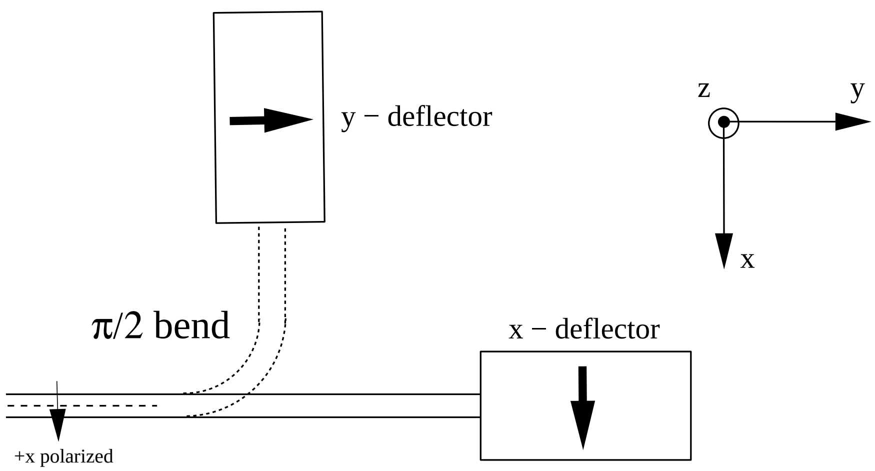

FIG. 3. An adjustable deflector.

The construction of s_y by appealing to orthogonal "thought" experiments is a bit tricky but contains this final crucial piece of information. Suppose we consider a beam of spins polarized in the x-direction that enters a tube with an x-deflector at the end of it. The tube is flexible and made of a material that does not interact with the magnetic moment or spin angular momentum (they are always proportional). Bending the tube by $\pi/2$ gives us a y-deflector setup (see figure 3). Bending the tube by π gives us a $-x$-deflector setup (see figure 4). We know the result of the experiment in π configuration: it is deflected "down" with respect to the deflector axis. Therefore the state entering this apparatus must have been: $|\uparrow\rangle_z - |\downarrow\rangle_z$. Comparing to the initial state $|\uparrow\rangle_x = |\uparrow\rangle_z + |\downarrow\rangle_z$, evidently the "bend" through the angle π affected the phase of the state $|\downarrow\rangle_z$ changing it from $+1$ to -1 [4].

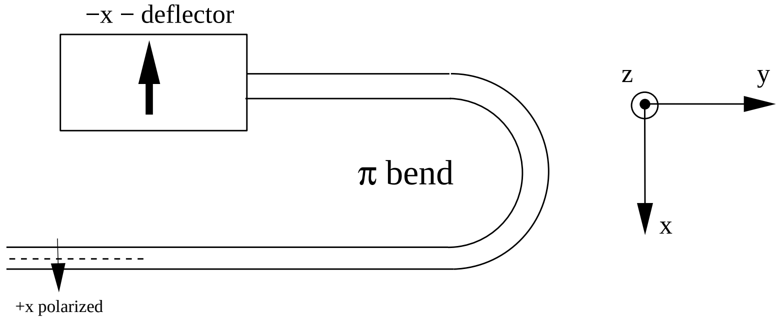

FIG. 4. An adjustable deflector in the π bend configuration.

What about a deflector set at the $\pi/2$ configuration (a y-deflector)? Let us generalize the superposition between $|\uparrow\rangle_z$ and $|\downarrow\rangle_z$ to include some relative phase:

$$e^{-i\theta/2}|\uparrow\rangle + e^{i\theta/2}|\downarrow\rangle$$

The π bend seems to be explained by setting $\theta = \pi$. If we assume that the phases depend linearly upon the angle of bend, then the y polarized state must be

$$|\uparrow\rangle_y = |\uparrow\rangle_z + i|\downarrow\rangle_z \qquad |\downarrow\rangle_y = |\uparrow\rangle_z - i|\downarrow\rangle_z$$

ignoring a global phase. Again, we deduce the hermitian operator corresponding to y polarization, s_y, from its eigenstates $|\uparrow\rangle_y$ and $|\downarrow\rangle_y$ (and eigenvalues $\pm\frac{1}{2}$):

$$s_y = \frac{1}{2}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$$

Relying only upon the discreteness of the vector space and the phenomenon of "orthogonal measurements" a complete set of observables has been constructed. Remarkably, these x, y, z-polarization operators form a Lie algebra with the following commutation relations:.

$$[s_i, s_j] = i\epsilon_{ijk}s_k \quad \epsilon_{ijk} = 1(-1) \text{ for even (odd) perm of 123} \tag{2}$$

This "quantization condition" is usually taken as the starting point of quantum mechanics, but it is nice to see rather physically how it arises. Larger spin ($S > \frac{1}{2}$) just corresponds to larger ($2S + 1 > 2$) dimensional representation of (2).

II. ARBITRARY SPIN AND THE MAJORANA REPRESENTATION

Ettore Majorana wrote a fascinating paper in 1932 [5] outlining a connection between the quantum mechanics of large spin and a special polynomial. This work has remained almost completely obscure for 69 years; as far as we know the paper has never been translated from Italian and Majorana himself disappeared in 1938 [6]. The work was recently resurrected by Roger Penrose in connection with the Bell inequality and non-locality [7].

The quantum mechanics of larger (than 1/2) spin corresponds to higher dimensional representations of the algebra defined by equation (2). The basis vectors for a spin-S space are denoted by $|m\rangle$ and m runs from $-S$ to S in integer steps. The basis vectors are chosen to be the eigenstates of s_z and thus:

$$s_z|m\rangle = m|m\rangle$$

Consider an arbitrary normalized state

$$a_{2S}|S\rangle + a_{2S-1}|S-1\rangle + a_{2S-2}|S-2\rangle + \ldots + a_0|-S\rangle$$

To this state, Majorana associates a polynomial

$$P(z) = c_n z^n + c_{n-1} z^{n-1} + \ldots + c_0$$

where $n \equiv 2S$ and the coefficients $c_j = B_j^{1/2} a_j$ where B_j is the binomial coefficient $B_j = n!/(n-j)!j!$. If the zeroes of $P(z)$ are computed and stereographically projected on the Riemann sphere, they have a special significance when regarded as *directions in real space for a "deflection" type measurement* as described in the previous section. Suppose the zeroes are given by the set $\{\alpha_j\}$, that is

$$P(z) = (z - \alpha_n)(z - \alpha_{n-1}) \ldots (z - \alpha_1) = 0 \qquad z \to z e^{i\theta/2} \quad \alpha_j \to \alpha_j e^{-i\theta/2}$$

Specifically, if any zero is chosen and a deflection measurement is made along the "direction" indicated by the point on the Riemann sphere, the measurement yields no deflections corresponding to the state $|-S\rangle$ (see figure 5).

For spin 1/2, since there are only two states, knowing that the antipodal measurement yields zero tells you the direction of polarization. For higher spin, an arbitrary state does not have a single "direction of polarization." There are many such directions. Lastly, the phase factors that the wavefunction acquires under parallel transport (used in our construction of hermitian operators) involve a transformation of z and α_j: they are shown to the right of the equation above.

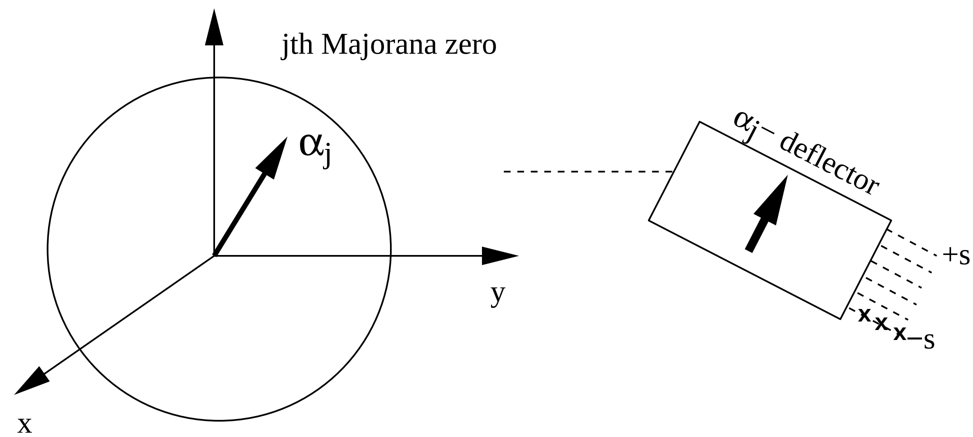

FIG. 5. One of the Majorana zeroes (α_j) and deflector adapted for measurement along that direction.

III. (LACK OF) APPLICATIONS

It is not clear that the Majorana representation is actually "useful" for anything. However, it is *a complete visual depiction of the wavefunction* as opposed to a probability distribution of some sort. It carries complete quantum information about the state of the system and is, in some sense, a generalization "polarization direction".

In quantum mechanics there is the cherished notion of the "correspondence principle" which states that when the action [8] becomes large relative to the Planck constant $\hbar$, the calculations of quantum mechanics and that of classical mechanics should coincide. Naively, one might expect that when S is large, the Majorana zeroes "cluster" along a direction that represents the classical angular momentum orientation, as the action is closely related to angular momentum.

Consider a hamiltonian of the form

$$H = -J_1 s_z^2 + J_2 s_x^2 \quad \longleftrightarrow \quad E(\theta, \phi) = -J_1 \cos\theta^2 + J_2 \sin\theta^2 \cos\phi^2 \tag{3}$$

This hamiltonian describes a quantum spin S: $s_{x,y,z}$ obey the same commutator, but a $2S+1$ dimensional representation is chosen. (The molecular magnets Fe_8 and Mn_{12} are $S = 10$ representatives.) Classically, the spin wants to point along the $\pm z$-axis but is energetically forbidden from crossing between the two "easy" directions, as depicted in figure 6.

Specifically, in the $S \to \infty$ limit, spin dynamics is well described by a Feynman path integral evaluated semiclassically, that is, close to the classical least action trajectory. Parameterizing the spin axis by spherical coordinates (θ, ϕ), the imaginary time (Euclidean) path integral is:

$$Z = \int [D\theta][D\phi] e^{-\int d\tau \{ iS\partial_\tau \phi (1-\cos\theta) + E(\theta,\phi)\}}$$

The $iS\partial\phi$ term represents the Berry phase and gives rise to the aforementioned non-holonomy for half-integer S.

For a typical hamiltonian H with an energy barrier there is an "instanton" solution and spin can cross the classically forbidden region and tunnel between $+z$ and $-z$ (figure 6). In the Majorana picture, one might expect that the zeroes of Majorana polynomial would "cluster" and follow the instanton trajectory over the energy barrier. To our surprise, this is not at all what happens.

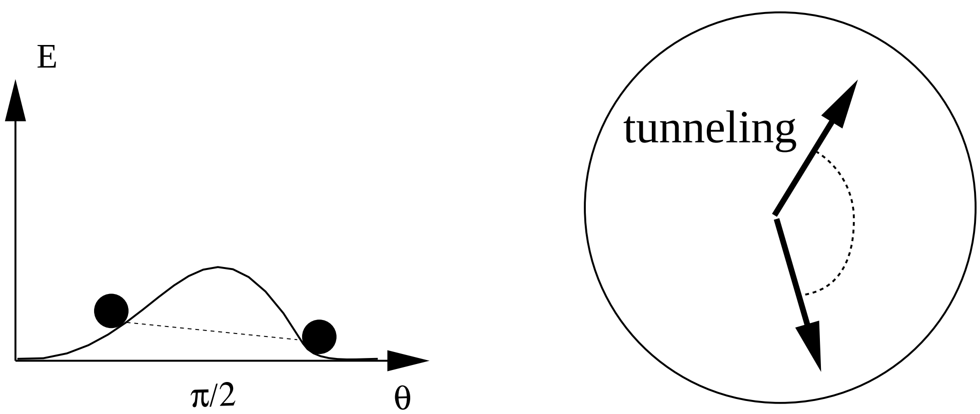

FIG. 6. Energy barrier for tunneling.

To study the dynamics of the zeroes we found (numerically) the time evolution of a particular initial prepared state and computed the zeroes of the Majorana polynomial (numerically) at small time intervals. The initial state was taken to be polarized in the $+z$ direction.

Schematically, the steps were: (1) Find the eigenstates of H (which are themselves some linear combinations of the basis vectors $|m\rangle$.) (2) Project the initial state onto eigenstates of H. (3) Evolve each component eigenstate in time. (The unitary evolution operator (1) is diagonal in this basis, so each component simply acquires a time dependent phase.) (4) Construct the Majorana polynomial at a given time and find its zeroes.

Figure 7 shows the zeroes of the Majorana polynomial corresponding to each of the sixteen eigenstates of H for $S = 8$. The zeroes are depicted by first projecting them onto the Riemann sphere and then vertically projecting them onto the plane. The procedure above then amounts to finding the zeroes of a polynomial of the form:

$$Q(z,t) = \sum_j e^{-i\epsilon_j t} w_j (z - \alpha_n^j)(z - \alpha_{n-1}^j) \dots (z - \alpha_1^j)$$

where each of the product terms represents an eigenstate component with weight w_j and energy eigenvalue ϵ_j. $\{\alpha_i^j\}$ is the set of zeroes of the jth eigenstate.

The following sequence of plots (figure 8) shows the time evolution of the zeroes as described by equation (1). The initial state at $t = 0$ is polarized in the $+z$ direction; accordingly, the zeroes are clustered at the north pole. Times are referenced to the period T of one tunneling event.

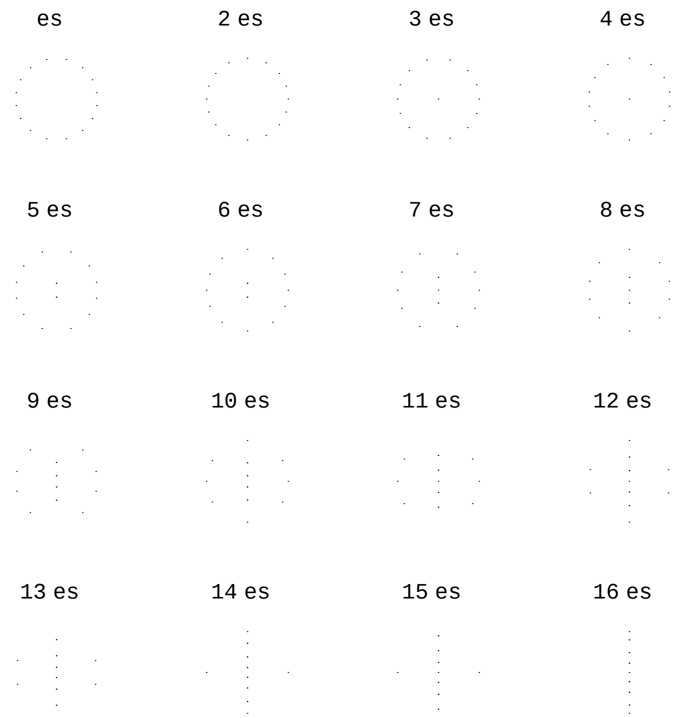

FIG. 7. Zeroes corresponding to eigenstates of H. Zeroes are projected onto the Riemann sphere then vertically projected back onto the plane.

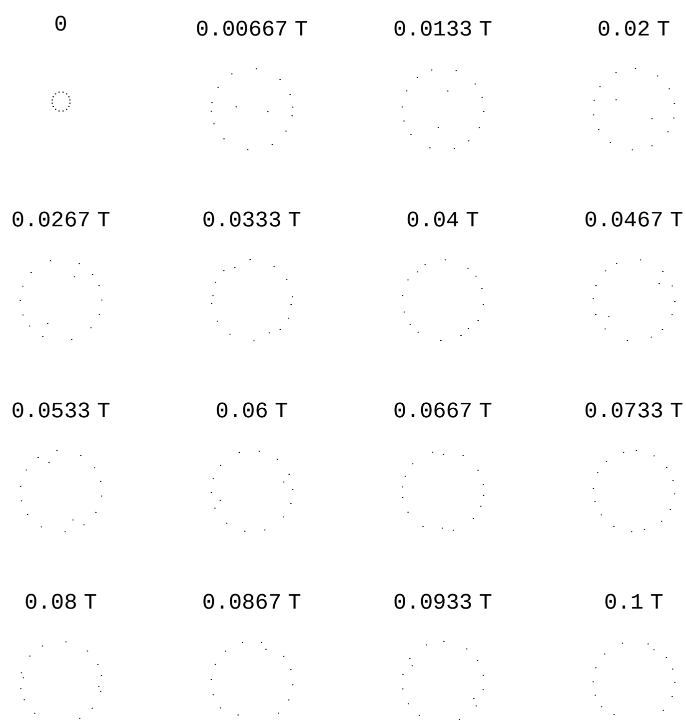

FIG. 8. Short time evolution of the zeroes.

After a short transient period, the zeroes are seen to spread out and migrate to the unit circle (the equator on the Riemann sphere.) However, notice that two "dissident" points have remained close to the unit circle but within it (in the northern hemisphere.)

Figure 9 depicts the short time dynamics of the tunneling event itself, at times $t \sim T/2$. Vertical projection onto the plane eliminates the north-south hemisphere information, but in the first five snapshots of figure 9, the two "dissident" zeroes are in the northern hemisphere. In the remaining eleven snapshots, the dissident zeroes are in the southern hemisphere. The tunneling event occurred (in the "Majorana" sense) between $t = 0.495T$ and $t = 0.497T$. The two dissidents will remain in the southern hemisphere until a second tunneling event, in the proximity of $t \sim T$, brings them back to the north.

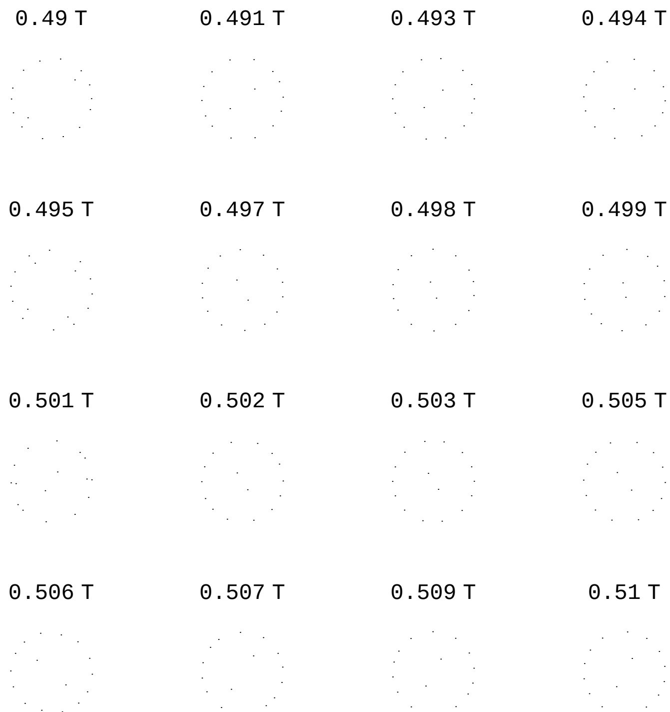

FIG. 9. Short time evolution of the zeroes during a tunneling event. The tunneling event takes place when the two "dissident" zeroes cross the equator between $t = 0.495T$ and $t = 0.497T$. The remaining frames show the dissisents in the southern hemisphere.

IV. CONCLUSION

We have presented here the first calculations of the dynamics of large spin using the Majorana polynomial. At first glance, these calculations suggest a picture quite different from the expected semiclassical physics of large spin. The zeroes of the Majorana polynomial do not cluster along a well defined polarization direction. Rather, all of the interesting dynamics is contained in the behavior of just two "dissident" zeroes (out of the all $2S = 16$ zeroes). The time at which the two dissidents cross the equator and visit the southern hemisphere is well correlated with the tunneling time obtained by the "instanton" approximation of the Feynman path integral.

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[1] * If you saw the asterisk and came here looking for a footnote, I will take the opportunity to tell you that (1) chemists use the * notation for excited state and (2) physicists use $|\rangle$ and $\langle|$ as notation for elements of vector space and dual space, respectively.

[2] We could choose basis vectors other than $|m\rangle, |m^*\rangle$. For instance, the linear combination $\frac{1}{\sqrt{2}}(|m\rangle \pm i|m^*\rangle)$. But there is no guarantee that a *simple* measurement corresponds to these two states.
[3] The $\frac{1}{2}$ because electrons carry $\frac{1}{2}\hbar$ units of angular momentum.
[4] This is in fact a Berry phase leading to a non-holonomic process. The phase factor described above is the connection under parallel transport of a spinor object.
[5] E. Majorana, Nuovo Cimento **9**, 43-50 (1932).
[6] During his very short career as a physicist, Majorana was regarded as an extraordinary talent. Enrico Fermi, one of the great physicists of the 20th century was quoted as saying (about Majorana): "There are different sorts of scientists. There are second and third rate scientists who do their best but don't go far. Next, there are first rank fellows in science who make discoveries of considerable importance... But then there is genius, like Galileo and Newton. Well I think Ettore Majorana was in that company."
[7] J. Zimba and R. Penrose, Stud. Hist. Phil. Sci. **24(5)**, 697-720 (1993).
[8] Action is a quantity from classical mechanics; for a mechanical system of a point particle of mass m in a potential $V(x)$, the action is: $S(t_i, t_f) \equiv \int_{t_i}^{t_f} (\frac{1}{2}m(\partial_t x)^2 - V(x))dt$ where the integral is taken over the classical trajectory of the particle $x(t)$.