Möbius Molecules, Pythagorean Triples and Fermat's Last Theorem

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It is shown that if a triple of distinct positive integers (a, b, c) were to exist such that $a^n + b^n = c^n$ for some odd integer $n \geq 3$, then it must be Pythagorean, i.e. $a^2 + b^2 = c^2$ must hold too, from which a contradiction arises since this is possible only if either a or b are zero. We arrive at this conclusion by investigating the (partial) trace of a model hamiltonian operator whose energy levels correspond to those of the so-called Hückel hamiltonian applied to rings containing an odd number of atoms lying on a Möbius strip rather than a planar topology. Furthermore, the contradictory nature of our result implies the correctness of the associated statement contained in the famous Fermat's Last Theorem. Given the use of concepts from quantum mechanics and matrix algebra unknown at his time, and the fact that the essence of the present proof may not fit within a margin of a typical book, mystery still remains over Pierre de Fermat's *demonstrationem mirabilem*.

A partial proof of his famous "Last Theorem" is due to Fermat himself, who had already established that the conjecture was true for the case of all exponents n that are either even numbers or non-prime odd numbers. In this work, we build a quantum mechanical model of non-interacting electrons for which the energy levels can be related to the statement of Fermat's Last Theorem at $n \geq 3$ odd.

Our quantum mechanical system is defined in terms of an odd number of states $n \geq 3$ that can be occupied each by at most two electrons (with opposite spins). Given the integer quantum numbers (a, b, n, k), with $b > a \geq 0$, we construct the set of quantum states denoted as $|a, b\zeta_n^k\rangle$ where $\zeta_n^k = e^{i\frac{2\pi k}{n}}$ is the corresponding n-th root of unity $(k = 0, 1, \ldots, n-1)$. These n states are connected through the action of the cyclic ladder operator

$$\hat{Z}_n^+ \; |a, b\zeta_n^k\rangle \;=\; (a + b\zeta_n^{k+1}) \; |a, b\zeta_n^{k+1}\rangle \; , \qquad (1)$$

and its adjoint

$$\hat{Z}_n^- \; |a, b\zeta_n^k\rangle \;=\; (a + b\zeta_n^{-k}) \; |a, b\zeta_n^{k-1}\rangle \; , \qquad (2)$$

built upon the relation $(\zeta_n^l)^* = \zeta_n^{-l}$. Due to the fact that $\zeta_n^{k\pm n} = \zeta_n^k$, only n distinct states exist for each pair (a, b), and these are moreover assumed to be orthonormal (i.e. $\langle a, b\zeta_n^k | a', b'\zeta_n^{k'}\rangle = \delta_{aa'}\delta_{bb'}\delta_{kk'}$). The ket $|a, b\zeta_n^k\rangle$ represents an eigenstate of the following one-particle hamiltonian operator:

$$\hat{H}_n \;=\; \hat{Z}_n^+ \hat{Z}_n^- \; , \qquad (3)$$

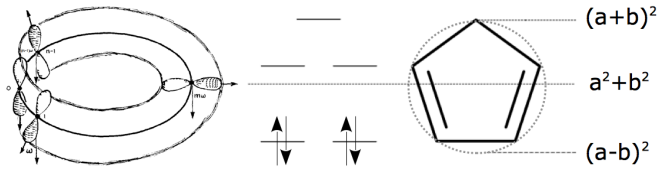
satisfying the eigenvalue equation

$$\hat{H}_n |a, b\zeta_n^k\rangle = (a + b\zeta_n^{-k})(a + b\zeta_n^k) |a, b\zeta_n^k\rangle \; . \qquad (4)$$

The expression $E_{ab}(k) = (a + b\zeta_n^{-k})(a + b\zeta_n^k)$ for the energy eigenvalue of the state $|a, b\zeta_n^k\rangle$ just obtained can be further cast into the form:

$$\begin{aligned} E_{ab}(k) \;&=\; a^2 + b^2 + ab(\zeta_n^k + \zeta_n^{-k}) \\ &=\; a^2 + b^2 + 2ab\cos\frac{2\pi k}{n} \; , \end{aligned} \qquad (5)$$

with each level being doubly degenerate, except for the highest level ($k = 0$). The following figure shows the diagram of the energy levels for the case of $n = 5$, and with a total of $N = 4$ electrons occupying the lowest levels according to the aufbau principle:



Our model hamiltonian produces actually the same pattern of energy levels of the Hückel hamiltonian[1] except for the completely reversed energetic order. In the example above, we see such pattern for a five-atom regular lattice representative of a cyclopentadienyl structure with four valence electrons. In a planar topology, the pattern would see the nondegenerate state as lowest in energy. However, when the topology of the lattice is that of a Möbius strip, a reversal of the energy ordering of the type shown in the above figure is to be expected.[2] Such "Möbius molecules" are absent in nature, but a handful of them have been synthesized in the laboratory, and their structures are not completely uncommon as chemical reaction intermediates.[3] The Hückel model is specified in terms of two physical parameters: the on-site/atomic energy α and the hopping parameter β (resonance integral) between two adjacent atoms, that measures the energy of stabilization experienced by an electron allowed to delocalize. The value of β between an atom and the next is modulated by a factor $\cos\omega$, where $\omega = \pi/n$ is the relative angle of the atomic orbitals as seen in the above figure (such angle would be zero in the corresponding planar topology). The connection with our model is made clear by means of the assignments $\alpha = a^2 + b^2$ and

$\beta\cos\omega = ab$, albeit for applications to molecules such parameters are usually both non-integer (and negative, as by the typical choice of the zero of the energy). As expected, our model predicts a stable electronic configuration upon delocalization of the four electrons across the lattice, as compared to the localized (atomic) states - the latter occupying an energy level standing at a^2+b^2. Such stabilization, known as aromaticity, would follow the "$4N$ rule" in this case, as opposed to the "$4N+2$ rule" for cyclic molecules that are planar.

Returning to the connection with Fermat's Last Theorem, we observe that Eq. (5), combined with the well-know identity $\sum_{l=0}^{n-1}\zeta_n^l = 0$ and its complex conjugate, gives the following result for the trace of our "Möbius hamiltonian" $\hat{H}_n$ in the (a,b) subspace:

$$\mathrm{Tr}_{(a,b)}\hat{H}_n \;=\; (a^2+b^2)n\;. \tag{6}$$

Next we investigate the eigenvalues of the operator $\hat{Z}_n^+$ by inspection of its matrix representation for the simplest case of $n = 3$. In the standard basis $|a,b\zeta_3\rangle = \{|a,b\zeta_3^0\rangle, |a,b\zeta_3^1\rangle, |a,b\zeta_3^2\rangle\}$, we have

$$\mathbf{Z}_3^+ \;=\; \begin{pmatrix} 0 & 0 & a+b \\ a+b\zeta_3 & 0 & 0 \\ 0 & a+b\zeta_3^2 & 0 \end{pmatrix} \;=\; \mathbf{D}_3\mathbf{P}_3\;, \tag{7}$$

and in general $\mathbf{Z}_n^+ = \mathbf{D}_n\mathbf{P}_n$, where the diagonal matrix $\mathbf{D}_n$ has elements: $(a+b),(a+b\zeta_n),\ldots,(a+b\zeta_n^{n-1})$, whereas $\mathbf{P}_n$ is the appropriate $n\times n$ cyclic permutation matrix. For the operator $\hat{Z}_n^-$, we get the hermitian transposed matrix, hence $\mathbf{Z}_n^- = \mathbf{P}_n^T\mathbf{D}_n^\dagger$. At this stage, we recognize the following relation: $\det(\mathbf{D}_n) = \prod_{k=0}^{n-1}(a+b\zeta_n^k) = a^n+b^n$, where the last identity is well-known and valid for n odd. With this result, the n eigenvalues of the ladder operators $\hat{Z}_n^+$ and $\hat{Z}_n^-$ can be easily shown to be of the form $c\zeta_n^m$ and $c\zeta_n^{-m}$, respectively, with $m = 0,\ldots,n-1$ and $c = \sqrt[n]{a^n+b^n}$. Furthermore, *if we assume c to be a positive integer*, this leads rather naturally to a second expression for the trace of the hamiltonian, namely

$$\mathrm{Tr}_{(a,b)}\hat{H}_n \;=\; nc^2 \quad\Leftrightarrow\quad c\in\mathbb{N}\;. \tag{8}$$

In order to prove Eq. (8), we proceed as follows. For the pair (a,b) that supposedly produces an integer value of $c = \sqrt[n]{a^n+b^n}$ at a given n, define the matrix $\mathbf{\Theta} = \mathbf{Z}_n^+$ leading to a hamiltonian matrix written as $\mathbf{H} = \mathbf{\Theta}\mathbf{\Theta}^\dagger$. In the subspace $(0,c)$, the corresponding matrix representation of the $\hat{Z}_n^+$ operator reads $\mathbf{\Gamma} = c\zeta\mathbf{P}_n$ where ζ is the diagonal matrix of the n-th roots of unity. By the assumption on the integer nature of c, the two matrices $\mathbf{\Theta}$ and $\mathbf{\Gamma}$ are similar, i.e. there exists a nonsingular matrix $\mathbf{X}$ such that $\mathbf{\Theta} = \mathbf{X}\mathbf{\Gamma}\mathbf{X}^{-1}$. As shown in the Supplementary Note, due to the peculiar structure of the matrices involved, this assumption leads to Eq. (8). Here we point out that in the special case in which the two matrices were to satisfy unitary equivalence, namely if $\mathbf{X}^{-1} = \mathbf{X}^\dagger$, the following relation alone $\mathrm{Tr}(\mathbf{H}) = \mathrm{Tr}(\mathbf{\Theta}\mathbf{\Theta}^\dagger) = \mathrm{Tr}(\mathbf{X}\mathbf{\Gamma}\mathbf{\Gamma}^\dagger\mathbf{X}^\dagger)$ would give straighforwardly Eq. (8) due to the invariance of the trace upon circular shifts.

By comparing Eq. (6) and Eq. (8), it follows that the relation $a^2+b^2 = c^2$ must be true, but since by definition $a^n+b^n = c^n$, the fulfillment of both relations would require either a or b to be zero. We then conclude that $c = \sqrt[n]{a^n+b^n}$ with a,b positive integers must always be irrational at $n\geq 3$ odd, in accordance with what Fermat conjectured sometime during the year 1637. (Q.E.D.)

In conclusion, the result presented here holds the missing piece to an elementary proof of what has come to notoriety as Fermat's Last Theorem. As such, it complements the important results occurred since the 17th century and culminating in the 1995 proof by Andrew Wiles.[4] The developments in many areas of mathematics that led to his proof are the truly significant results of the endeavours of the many mathematicians who worked on the problem. What presented here is instead an answer to Fermat's question whereby little or no progress in mathematics is expected. It is a blessing that such a proof - or one alike, if indeed Pierre de Fermat kept it undisclosed - remained lost for centuries. Perhaps the greatest gift to mankind from the man himself.

Addendum. The central result of this work can be restated as follows: given $b > a \geq 0$ integers that identify the bound states $|\psi(a,b)\rangle$ of a quantum particle, no such state can exist of the type $|\psi(0,c)\rangle$ if $c^n = a^n+b^n$ for some $n\geq 3$ odd integer (and for $a\neq 0$). The existence of such a state would in fact give rise to the following contradiction: by defining a hermitian model based on the Möbius hamiltonian $\hat{H}_n$ of Eq. (3), where the states $|\psi\rangle$ are augmented with a set of what we may call "Möbius spin" states $|\chi(s,m_s)\rangle_{m_s=-s,\ldots,s}$, with $n = 2s+1$ to form the eigenstates $|a,b\zeta_n^k\rangle = |\psi(a,b)\rangle|\chi(s,k-n)\rangle$ of $\hat{H}_n$, it is shown that $c^2 = a^2+b^2$ must also be true, which is a *reductio ad absurdum*.[5] Given that the initial quantum system, except for the requirements of admitting normalizable wavefunctions and a discrete energy spectrum - as it is the case for any spatially confined hermitian system - can be completely arbitrary, and therefore a,b and c map nonnegative integers, this is a restament of Fermat's Last Theorem in terms of the triple (a,b,c) for n odd.

I. SUPPLEMENTARY NOTE

The matrices $\mathbf{\Gamma}$ and $\mathbf{\Theta}$ are both examples of cyclic monomial matrices.[6] Based on their peculiar properties, we will first prove that a matrix $\mathbf{X}$ performing the similarity transformation $\mathbf{\Theta} = \mathbf{X}\mathbf{\Gamma}\mathbf{X}^{-1}$ can be chosen to be a diagonal matrix. Setting $\mathbf{\Theta} = \mathbf{D}_n\mathbf{P}_n$ and $\mathbf{\Gamma} = \mathbf{G}_n\mathbf{P}_n$, we can write the assumed similarity relation as follows:

$$\mathbf{D}_n\mathbf{P}_n = \mathbf{X}(\mathbf{G}_n\mathbf{P}_n)\mathbf{X}^{-1} = (\mathbf{X}\mathbf{G}_n\tilde{\mathbf{X}}^{-1})\mathbf{P}_n\;, \tag{9}$$

where $\tilde{\mathbf{X}}^{-1} = \mathbf{P}_n\mathbf{X}^{-1}\mathbf{P}_n^T$ is again a diagonal matrix with the nonzero elements cyclically shifted. In particular, if

we indicate by $\{x_k | k = 0, \ldots, n-1\}$ the diagonal elements of $\mathbf{X}$, then $(\tilde{X}^{-1})_{kk} = 1/x_{k-1}$, where it is understood that "$k = -1$" means "$k = n-1$" as for the type of modular arithmetic implied in our reasoning. The sought-for similarity transformation is then accomplished by a diagonal matrix $\mathbf{X}$ satisfying the equation $\mathbf{X}\mathbf{G}_n\tilde{\mathbf{X}}^{-1} = \mathbf{D}_n$, i.e. with diagonal elements that fulfill the recursive relation

$$c\ \zeta_n^k\ x_k\ =\ (a + b\zeta_n^k)\ x_{k-1}\ , \tag{10}$$

where $k = 0, \ldots, n-1$ and $x_{-1} := x_{n-1}$. In the above equations, we can arbitrarily set $x_0 = 1$ without loss of generality, and at the same time guaranteeing that $\mathbf{X}$ is nonsingular, and hence invertible. Consequently, the following diagonal matrix $\mathbf{S} = \mathbf{X}^\dagger\mathbf{X}$ can be constructed from the recursive formula for its diagonal elements s_k :

$$c^2\ s_k\ =\ |a + b\zeta_n^k|^2\ s_{k-1}\ , \tag{11}$$

where $s_0 = 1$ and $s_{-1} := s_{n-1}$.

Next, consider the property of $\mathbf{\Gamma}$ being a normal matrix (i.e., $\mathbf{\Gamma}\mathbf{\Gamma}^\dagger = \mathbf{\Gamma}^\dagger\mathbf{\Gamma}$, as it can be easily shown by direct evaluation of the two matrix products in terms of the matrices $\mathbf{P}_n$ and ζ). It then follows that $\mathbf{\Gamma}$ is diagonalizable by means of a unitary matrix $\mathbf{U}$. At the same time, the diagonal matrix $\mathbf{G}_n$ has a particular structure: except for the diagonal element g_0 that is singled out, the other elements satisfy the relation $g_k = g^*_{n-k}$. In other words, $\mathbf{G}_n^\dagger = \mathbf{Q}_n\mathbf{G}_n\mathbf{Q}_n$ where the matrix $\mathbf{Q}_n$ is defined as follows:

$$\mathbf{Q}_n\ =\ \begin{pmatrix} 1 & \mathbf{0} \\ \mathbf{0} & \mathbf{J}_{n-1} \end{pmatrix}\ =\ \mathbf{Q}_n^T\ =\ \mathbf{Q}_n^{-1}\ , \tag{12}$$

where $\mathbf{J}_{n-1}$ is an orthogonal symmetric matrix ($\mathbf{J} = \mathbf{J}^T = \mathbf{J}^{-1}$) of dimension $n-1$ formed by 1's that reside on the antidiagonal and zeros for all other elements - often called the *reversal matrix*. The following chain of equalities is then established:

$$\mathbf{\Gamma}^\dagger = \mathbf{P}_n^T\mathbf{G}_n^\dagger = \mathbf{P}_n^T\mathbf{Q}_n^T(\mathbf{G}_n\mathbf{P}_n)\mathbf{P}_n^T\mathbf{Q}_n^T = \mathbf{J}_n\mathbf{\Gamma}\mathbf{J}_n\ , \tag{13}$$

where the equality $\mathbf{J}_n = \mathbf{Q}_n\mathbf{P}_n$ can be easily proven by inspection through block-wise multiplication. (Note that the same property holds for $\mathbf{\Theta}$, i.e. $\mathbf{\Theta}^\dagger = \mathbf{J}_n\mathbf{\Theta}\mathbf{J}_n$.) The normality condition for $\mathbf{\Gamma}$, combined with Eq. (13) can thus be recast to require the following matrix commutativity:

$$[\mathbf{\Gamma}, \mathbf{J}_n\mathbf{X}^{-1}\mathbf{\Theta}\mathbf{X}\mathbf{J}_n]\ =\ 0\ . \tag{14}$$

The above equation implies that the unitary matrix $\mathbf{U}$ that diagonalizes $\mathbf{\Gamma}$ defines a common eigenbasis with the matrix $\mathbf{J}_n\mathbf{X}^{-1}\mathbf{\Theta}\mathbf{X}\mathbf{J}_n$, and therefore

$$(\mathbf{U}^\dagger\mathbf{J}_n\mathbf{X}^{-1})\ \mathbf{\Theta}\ (\mathbf{X}\mathbf{J}_n\mathbf{U})\ =\ c\zeta^\dagger\ =\ \mathbf{Q}_n(c\zeta)\mathbf{Q}_n\ . \tag{15}$$

We have thus identified in $\mathbf{R} = \mathbf{X}\mathbf{J}_n\mathbf{U}\mathbf{Q}_n$ the matrix of right-eigenvectors of $\mathbf{\Theta}$. Furthermore, we readily obtain the crucial result that $\mathbf{R}\mathbf{R}^\dagger = \mathbf{X}\mathbf{X}^\dagger = \mathbf{S}^\dagger = \mathbf{S}$ *is itself a diagonal matrix*. This fact alone simplifies the calculation of the trace of $\mathbf{\Theta}\mathbf{\Theta}^\dagger$ in the basis of the right-eigenvectors of $\mathbf{\Theta}$, as

$$\mathrm{Tr}[\mathbf{\Theta}\mathbf{\Theta}^\dagger]\ =\ c^2\ \mathrm{Tr}[(\mathbf{R}^\dagger\mathbf{R})\zeta(\mathbf{R}^\dagger\mathbf{R})^{-1}\zeta^\dagger]\ =\ nc^2\ . \tag{16}$$

We have therefore shown that the assumption of $\mathbf{\Theta}$ and $\mathbf{\Gamma}$ being similar matrices leads to the possibility for the transformation matrix $\mathbf{X}$ such that $\mathbf{\Theta} = \mathbf{X}\mathbf{\Gamma}\mathbf{X}^{-1}$ to be of diagonal form. When this result is combined with Eq. (13) and the normality condition on $\mathbf{\Gamma}$, an expression for the right-eigenvectors of $\mathbf{\Theta}$ is obtained that is suitable to directly validate Eq. (8).

Our proof is now complete.

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[1] E. Hückel, *Zeitschrift für Physik*, 70, 204 (1931); 72, 310 (1931); 76, 628 (1932); 83, 632 (1933).

[2] E. Heilbronner, *Tetrahedron Letters*, 5: 19231928 (1964).

[3] R. Herges, *Chemical Reviews*, 106: 48204842 (2006).

[4] A. Wiles, *Annals of Mathematics*, 141(3), 443 (1995).

[5] An example of such bound states $|\psi(a,b)\rangle$ are the hydrogenic wavefunctions, with b representing the principal quantum number, a the quantum number l of the angular momentum operator $\hat{L}^2$, and with a given $\hat{L}_z$ component, e.g., that with the magnetic number $m_l = 0$. In the real-space lattice model we would place n such wavefunctions along the Möbius strip one after the other at a fixed relative angle $\omega = \pi/n$, and then diagonalize the proper nearest-neighbour hamiltonian (noticeably, the cartoon of the cyclopentadienyl on a Möbius topology refers to the case in which $b = 2$ and $a = 1$, with a representation of the so-called $2p_0$ atomic orbitals along the strip). In our model, we use instead any arbitrary set of $n = 2s+1$ orthonormal functions $|\chi(s, m_s)\rangle$, akin to adding an extrinsic (Möbius) spin degree of freedom, i.e. they are the eigenfunctions of two new operators, $\hat{\mathcal{M}}^2$ and $\hat{\mathcal{M}}_z$, of angular momentum type - to form the eigenstates $|a, b\zeta_n^k\rangle$ of $\hat{H}_n$ directly.

[6] A monomial, or scaled permutation matrix $\mathbf{M}$ has the form $\mathbf{M} = \mathbf{D}\mathbf{P}$ where $\mathbf{D}$ is a nonsingular diagonal matrix and $\mathbf{P}$ a permutation matrix. As by the orthogonality of $\mathbf{P}$, monomial matrices satisfy a relation akin to commutativity, namely $\mathbf{D}\mathbf{P} = \mathbf{P}\mathbf{P}^T\mathbf{D}\mathbf{P} = \mathbf{P}\tilde{\mathbf{D}}$ where $\tilde{\mathbf{D}} = \mathbf{P}^T\mathbf{D}\mathbf{P}$ is simply $\mathbf{D}$ with the diagonal elements reordered. Finally, the characteristic equation for the eigenvalues λ of a cyclic monomial matrix $\mathbf{M} = \mathbf{D}\mathbf{P}$, hence whenever $\mathbf{P}$ is specifically a cyclic permutation, reads for n odd: $\lambda^n - \det(\mathbf{D}) = 0$. [see, J.L. Stuart and J.R. Weaver, *Linear Algebra Appl.*, 212/213 (1994), 397]