Möbius Molecules, Pythagorean Triples and Fermat's Last Theorem

Francesco Aquilante
Email: francesco.aquilante@gmail.com
Theory and Simulation of Materials (THEOS), and National Centre for Computational Design and Discovery of Novel Materials (MARVEL), École Polytechnique Fédérale de Lausanne, CH-1015 Lausanne, Switzerland
(Dated: July 4, 2024)

It is shown that if a triple of distinct natural numbers (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 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, made here but 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 fermionic particles 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), 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 ($k = 0, 1, \dots, n-1$). These n states are connected through the action of the cyclic ladder operator

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

and its adjoint

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

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 a given set (a, b, n), and these are moreover assumed to form an orthonormal basis for the corresponding Hilbert space (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:

$$\hat{H}_n \;=\; \hat{Z}_n^+ \hat{Z}_n^- \;, \tag{3}$$

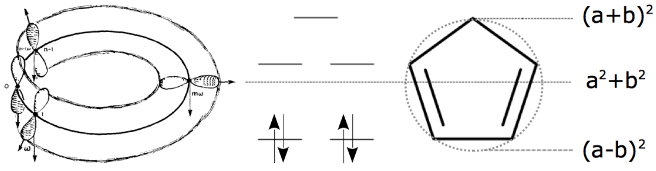
satisfying the eigenvalue equation

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

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:

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

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 non-degenerate 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 on a plane.

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 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 $\mathbf{Z}_n^- = \mathbf{P}_n^T\mathbf{D}_n^*$. 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), the operator $\hat{Z}_n^-$ gives rise to a non-hermitian matrix for which a right $|\mathcal{R}_m(a,b)\rangle$ and a left eigenvector $|\mathcal{L}_m(a,b)\rangle$ exist at each eigenvalue $c\zeta_n^{-m}$. Biorthogonality gives $\langle\mathcal{L}_k(a,b)|\mathcal{R}_m(a,b)\rangle = \delta_{km}$, but no such constraints hold for the norm of the eigenvectors. Hence, the trace condition $(a^2+b^2)n = c^2\sum_m\langle\mathcal{R}_m(a,b)|\mathcal{R}_m(a,b)\rangle$ results from expressing the trace in the right-eigenvector basis: $\mathrm{Tr}_{(a,b)}\hat{H}_n = \sum_m(\hat{Z}_n^-|\mathcal{R}_m(a,b)\rangle)^\dagger(\hat{Z}_n^-|\mathcal{R}_m(a,b)\rangle)$. However, if c is an integer then another set of eigenstates of $\hat{Z}_n^-$ are found to have the same set of eigenvalues $c\zeta_n^{-m}$, being the states $|\mathcal{R}_m(0,c)\rangle$ obtained in the subspace of the basis states $|0, c\zeta_n^k\rangle$, and therefore orthogonal to the basis states $|a, b\zeta_n^k\rangle$.

By the principle of superposition, states of the type $|\psi_m\rangle = \mu_m|\mathcal{R}_m(a,b)\rangle + \nu_m|\mathcal{R}_m(0,c)\rangle$ are then legitimate eigenstates with the same eigenvalue as its two components whenever $\mu_m^2 + \nu_m^2 = 1$ (to preserve biorthogonality). For the sake of our proof, we will consider the specific case in which the coefficients μ_m and ν_m are chosen to be independent from m. In this case, the trace in the larger space $|\mathcal{R}(a,b)\rangle \oplus |\mathcal{R}(0,c)\rangle$ reads:

$$\begin{aligned} \mathrm{Tr}_\psi \hat{H}_n \;&=\; \mu^2c^2\sum_m\langle\mathcal{R}_m(a,b)|\mathcal{R}_m(a,b)\rangle \\ &+\; \nu^2c^2\sum_m\langle\mathcal{R}_m(0,c)|\mathcal{R}_m(0,c)\rangle \\ &=\; \mu^2(a^2+b^2)n \;+\; \nu^2nc^2 \; . \end{aligned} \tag{9}$$

On the other hand, when expressed in the direct sum of basis states $|a, b\zeta_n\rangle \oplus |0, c\zeta_n\rangle$, the same trace is given by $(a^2+b^2)n + nc^2$, and *the two expressions should coincide for any choice of the coefficients μ and ν satisfying the constraint $\mu^2+\nu^2 = 1$*. But this appears to be possible only if the relation $a^2+b^2 = c^2$ holds. (Q.E.D.)

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 $c = \sqrt[n]{a^n+b^n}$ must always be irrational, in accordance with what Fermat conjectured sometime during the year 1637.

Our proof is now complete.

Addendum. 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.

[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] Wiles, A. (1995). Modular Elliptic Curves and Fermat's Last Theorem. Annals of Mathematics, 141(3), second series, 443-551. doi:10.2307/2118559