Molecular Knots and Links

Summary and References

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The development of knot theory, including some related developments in chemistry and physics. Part 1

1805 John Dalton (1766–1844): The modern atom hypothesis

before 1865 Some mathematicians and physicists make first steps towards the development of knot theory:
– Alexandre-Théophile Vandermonde (1735–1796)
– Carl Friedrich Gauß (1777–1855)
– August Ferdinand Möbius (1790–1868)
– Johann Benedikt Listing (1808–1882)
– James Clerk Maxwell (1831–1879)
The studies by Gauß and Maxwell were related to the development of electrodynamics, i.e. a theory for electricity and magnetism.
Listing is one of the founders of topology ('analysis situs').
Möbius discovered the Möbius strip in 1858 (in a document discovered only after his death), but Listing described this object earlier already.

1867/1869 Sir William Thomson (1824–1907, later to become Lord Kelvin / Joule-Thomson effect) proposes the 'vortex model' of the atom.
Inspiration for this model came from the work on hydrodynamics of vortex motion ("Hydrodynamik der Wirbelbewegung", 1858) by Hermann Ludwig Ferdinand Helmholtz (1821–1894), and from experiments on smoke rings by Peter Guthrie Tait (1831–1901).
J. C. Maxwell, being first quite reserved to Thomson's idea, finally accepts it because this atomic model satisfies all demands to a much larger extent than any other model considered so far.
If the vortex model of the atom is correct, then the understanding of matter on a microscopic scale requires the study of knots (and links).

1869 Dmitri Ivanovich Mendeleev (1834-1907) proposes the 'periodic' table of the chemical elements.

1877/1887 P. G. Tait and Thomas P. Kirkman (1806–1895) develop knot tables for alternating knots with up to 10 crossings. These tables also include some links (with two or three components).

1892 Hermann Brunn discusses links with n components which separate into the trivial link with $n-1$ components (i.e. into $n-1$ separate trivial knots) whenever any single component is removed. Links with this property are now called Brunnian links. A popular example is the Borromean link ($n = 3$).

1897 Joseph John Thomson (1856–1940) discovers the electron (cathode rays are beams of free electrons). When the electron is a constitutent of matter, then an atom likely contains electrons.

1899/1900 C. N. Little presents a knot table for non-alternating knots with 10 crossings (after six years of work).

1903 Emil Fischer (1852–1919, Nobel prize in Chemistry 1902) recognizes peptides and proteins as oligomers or polymers of α-amino acids, and synthesizes peptides for the first time

1906/1912 Experiments done by Ernest Rutherford (1871–1937, Nobel prize in Chemistry 1908), Hans Geiger (1882–1945), and Ernest Marsden (1889–1970) lead to a new model of the atom: A massive nucleus is surrounded by electrons (Rutherford's model).

This is the final stroke which turns Thomson's vortex model obsolete.

1908 Heinrich Tietze (1880–1964) states the conjecture that two different knots cannot have the same complement.

1912 Richard Willstätter (1872–1942, Nobel prize in Chemistry 1915) takes into consideration the possibility of existence of catenanes (carbon ring compounds of required size were not yet known!).

1914 Max Wilhelm Dehn (1878–1952) proves the inequivalence of right- and lefthanded forms of the trefoil knot.

1924/1926 Leopold Ružička (1887–1976, Nobel prize in Chemistry 1939 with Adolf Butenandt) identifies the fragrances civetone ($C_{17}H_{30}O$) and muscone ($C_{16}H_{30}O$) as macrocyclic ketones, and presents a method for their synthesis. Carbocyclic rings with up to about 35 atoms can be synthesized for the first time.

1927 M. Kerschbaum identifies the fragrance ambrettolide ($C_{16}H_{28}O_2$) as a macrocyclic lactone.

The development of knot theory, including some related developments in chemistry and physics. Part 2

1923 James W. Alexander (1888–1971): Every knot or link can be obtained from a closed braid (Theorem of Alexander, though an earlier proof has been given by H. Brunn already in 1897).

1925 Emil Artin (1898–1962) publishes the 'Theory of Braids'.

1925/1926 The birth of the new quantum mechanics: Matrix mechanics (Werner Heisenberg, 1901–1976, Nobel prize in Physics 1932) and wave mechanics (Erwin Schrödinger, 1887–1961, Nobel prize in Physics 1933 with Paul A. M. Dirac). The electronic structure of the one-electron atom can be understood for the first time. The spatial part of stationary state functions and associated eigenvalues are

$$\Psi_{nlm}(\mathbf{r}) = r^{-1}\, P_{nl}(r)\, Y_{lm}(\theta,\phi)\ , \qquad P_{nl}(r) = N_{nl}\, x^{l+1}\, \mathrm{e}^{-x/2}\, L_{n_r}^{(2l+1)}(x)$$

$$x = \frac{2Zr}{n}\ , \qquad n_r = n - l - 1\ , \qquad L_n^{(\alpha)}(x) = \sum_{k=0}^{n} (-1)^k \binom{n+\alpha}{n-k} \frac{x^k}{k!}$$

$$\widehat{\mathcal{H}}\Psi_{nlm} = E_n \Psi_{nlm}\ , \qquad E_n = -\frac{1}{2}\frac{Z^2}{n^2}\frac{e^2}{4\pi\varepsilon_0 a_0}\ , \qquad a_0 = \frac{4\pi\varepsilon_0\hbar^2}{m_\mathrm{e} e^2}$$

$$\widehat{\mathcal{L}}^2\Psi_{nlm} = l(l+1)\hbar^2\Psi_{nlm}$$

$$\widehat{\mathcal{L}}_z\Psi_{nlm} = m\hbar\Psi_{nlm}$$

The spectra of one-electron atoms are understood, i.e. the Lyman, Balmer, etc. series in case of hydrogen (except for finer details which require relativity, spin-orbit coupling, interaction of higher electric/magnetic multipole moments etc. to be included).

1926 Erwin Fues (1893–1970) applies the Schrödinger equation successfully to the problem of vibrational states of diatomic molecules (he uses the Kratzer potential, $V(R) = -A/R + B/R^2$, $A > 0$, $B > 0$ as effective internuclear potential).

1926 Kurt Reidemeister (1893–1971) introduces the three moves Ω_i, $i = 1, 2, 3$, for knot projections, now known as Reidemeister moves. These are sufficient to study any allowed deformation of a knot by studying the effects of these moves on the knot diagram.

1927 Walter Heitler (1904–1981) and Fritz London (1900–1954) apply the Schrödinger equation successfully to the ground state of the hydrogen molecule, $H_2\ X\ {}^1\Sigma_g^+$. Their wave function ansatz (valence bond ansatz) is

$$\Psi(1,2) = N\,\frac{1}{\sqrt{2}}\left\{\psi_a(\mathbf{r}_1)\psi_b(\mathbf{r}_2) + \psi_b(\mathbf{r}_1)\psi_a(\mathbf{r}_2)\right\}\frac{1}{\sqrt{2}}\left\{\alpha(1)\beta(2) - \beta(1)\alpha(2)\right\}$$

The 'covalent chemical bond' is understood for the first time.

1928 J. W. Alexander invents a polynomial invariant $\Delta(x)$ (now called Alexander polynomial) for knots and links.

1928/1929 Egil Andersen Hylleraas (1898–1965) applies the Schrödinger equation successfully to the ground state of the helium atom, He $X\ {}^1S$. The spatial part of his wave function ansatz depends explicitly on the interelectronic distance r_{12}. A simple example for such a function is

$$\Psi(\mathbf{r}_1,\mathbf{r}_2) = N\,\mathrm{e}^{-\zeta(r_1+r_2)}(1 + c r_{12})$$

The electronic structure of a two-electron atom is understood for the first time.

1932 K. Reidemeister publishes the first textbook on knot theory.

1933 Karl W. Ziegler (1898–1973, Nobel prize in Chemistry 1963 with Giulio Natta) and coworkers present a new, more efficient synthetic method for macrocyclic compounds from α,ω-dinitriles, based on earlier work (1912) by P. Ruggli (1884–1945). The technique is known now as Ruggli-Ziegler dilution principle.

The development of knot theory, including some related developments in chemistry and physics. Part 3

1934 Herbert Seifert (1907–1996): Every (oriented) knot represents the boundary line of an orientable surface in 3-space, the Seifert surface of the knot. Or, equivalently, to every given knot can be constructed an orientable surface in 3-space for which the knot represents the boundary line.

1935 J. Henry C. Whitehead (1904–1960) discovers the two-component link now bearing his name.

1944 Oswald Avery (1877–1955), Maclyn McCarty (1911–2005) and Colin M. MacLeod (1909–1972) provided experimental evidence that DNA is the substance responsible for heredity.

1947 Frederick Sanger (* 1918, Nobel prize in Chemistry 1958, and again 1980 [with Paul Berg and Walter Gilbert]) determines for the first time the amino acid sequences of a protein, of the protein insulin

1949 Horst Schubert proves the uniqueness of the decomposition of a knot into prime knots. A consequence of this proof is that there does not exist an inverse knot to any given knot, such that the composite knot formed from these two knots reduces to the trivial knot. This is completely different from the situation with braids!

1950 Erwin Chargaff (1905–2002) finds that the base composition in DNA is such that A=T and G=C, so that equal amounts pyrimidine and purine bases are present. In addition, the base composition of DNA varies from one species to another (Chargaff rules).

1951 Linus Pauling (1901–1994, Nobel prize in Chemistry 1954, Nobel Peace prize 1962), Robert C. Corey (* 1928, Nobel prize in Chemistry 1990), and H. R. Branson discover the α-helix structure (and Pauling and Corey also the β-sheet structure) of proteins

1951/1953 Rosalind Franklin (1920–1958) and Maurice Wilkins (1916-2005, Nobel prize in Medicine or Physiology 1958 with James D. Watson and Francis H. C. Crick) are involved in X-ray diffraction studies of DNA

1952 Joshua Lederberg (* 1925, Nobel prize in Medicine or Physiology 1958 with George Wells Beadle and Edward Lawrie Tatum) coins the term 'plasmid' for (in most cases) circular, extrachromosomal, double-stranded DNA molecules found mainly in bacteria, but also in some yeasts and fungi. As we know today, genes on plasmids are involved in or responsible for e.g. fertility or antibiotic resistance of these organisms.

1953 James D. Watson (* 1928) and Francis H. C. Crick (1916–2004) — both received the Nobel prize in Medicine or Physiology 1962 with Maurice H. F. Wilkins — identify a model structure of double-stranded DNA.

1954 Arthur Lüttringhaus (1906–1992) starts to work on a direct and controlled synthesis of a [2]-catenane.

1959 Bruce Merrifield (* 1921, Nobel prize in Chemistry 1984) invents the solid phase synthesis for peptides and (small) proteins

1960 Robert L. Sinsheimer and Walter Fiers discover that the genetic material of the bacterial virus ϕX174 is in the form of a ring of single-stranded DNA

1960 Edel Wasserman claims to have synthesized a [2]-catenane, but his claims cannot be confirmed (neither by himself nor by others).

1963 John Cairns first observes double-stranded DNA rings

1963 Jerome Vinograd (1913–1976) identifies supercoiled structure of DNA

1964 Gottfried Schill and A. Lüttringhaus report on the first successful controlled synthesis of a [2]-catenane.

1967 Jerome Vinograd and coworkers discover catenated forms of mitochondrial DNA in human tumor cells (HeLa cells and leukaemic leucocytes).

1967 John Horton Conway (* 1937) presents a new notation for knots and links, uses 'surgery' to derive the skein relation for oriented knots and links, and thus finds a new simpler way to determine the Alexander polynomial recursively. This Alexander-Conway polynomial of a knot or link L (also known as potential function of L), $\nabla_L(z)$, can be obtained recursively from the two relations

$$\nabla_{0_1}(z) = 1 \,, \qquad \nabla_{L_+}(z) - \nabla_{L_-}(z) + z\,\nabla_{L_0}(z) = 0$$

where the latter relation, the skein relation, involves oriented links L_+, L_-, and L_0 that differ in only one crossing (right-hand, left-hand, or no crossing). For a knot K, the Alexander-Conway polynomial $\nabla_K(z)$, with $z = t^{1/2} - t^{-1/2}$, is identical to the Alexander polynomial, $\Delta_K(t)$, normalized such that $\Delta_K(t) = \Delta_K(t^{-1})$ and $\Delta_K(0) = 1$]. Conway publishes a catalogue for prime knots with up to 11 crossings, and prime links with up to 10 crossings (without use of a computer, and with only a few errors).

1968 Stanley Cohen (* 1922, Nobel prize in Physiology or Medicine 1986) discovers plasmids, and their importance for antibiotic resistance of bacteria.

1971 Discovery of DNA topoisomerases by James C. Wang.

1974 Kenneth A. Perko, Jr., points out that the two knots 10_{161} and 10_{162} are actually only two representations of the same knot.

1977 DNA sequencing techniques become available

1982 David M. Walba and coworkers synthesize a molecular Möbius strip.

1983 C. Hugh Dowker (1912–1982) invents a new notation for knots which is suitable for computer implementation.

1983 Andrzej Stasiak, Theodor Koller, and coworkers develop a technique to cover DNA with a protein, the *recA* protein. This allows to deduce unequivocally the absolute handedness of DNA knots and catenanes from electron microscopic pictures.

1985 Kary B. Mullis (* 1944, Nobel prize in Chemistry 1993) invents the polymerase chain reaction (PCR), which allows to generate genetic material from a single molecule of double-stranded DNA

1985 Vaughan F. R. Jones (* 1952, Fields medal 1990) invents a new polynomial invariant $V(t)$ (now called Jones polynomial), which can distinguish a knot from its mirror image. The Jones polynomial may be calculated recursively from

$$V_{0_1}(t) = 1 \,, \qquad t^{-1}\,V_{L_+}(t) - t\,V_{L_-}(t) - z\,P_{L_0}(t) = 0 \,, \qquad z = t^{1/2} - t^{-1/2}$$

1985 The HOMFLY polynomial, a new polynomial invariant in two variables, $P_L(l,m)$, is discovered (the acronym combines the initial letters of some of the discoverers, Hoste, Ocneanu, Millett, Freyd, Lickorish, and Yetter; the acronym LYMPH-TOFU, proposed by the Israeli mathematician D. Bar-Natan to account for all known and unknown discoverers, did not succeed). The HOMFLY polynomial may be calculated recursively from

$$P_{0_1}(l,m) = 1 \ , \qquad l\, P_{L_+}(l,m) + l^{-1}\, P_{L_-}(l,m) + m\, P_{L_0}(l,m) = 0$$

1989 Cameron McA. Gordon and John Luecke prove the Tietze conjecture: Two knots are the same if and only if the space around them (their complement) is the same.

1989 Christiane Dietrich-Buchecker and Jean-Pierre Sauvage (* 1944) synthesize a molecular trefoil knot with a template technique based on transition metal complexes.

1990 Victor Vassiliev discovers the existence of hierarchies of knot invariants. This opens the way to use higher invariants, in case that simpler ones do not suffice to distinguish a given knot from another one.

1990/1991 Jean-Pierre Sauvage and coworkers synthesize $[n]$-catenanes ($n = 2, ..., 7$) with a template technique based on transition metal complexes.

1991 Nadrian C. Seeman and coworkers synthesize a single-stranded DNA trefoil knot, using the self-assembly properties of DNA

1994 J. Fraser Stoddart (* 1942), UCLA, synthesizes olympiadane, a [5]-catenane, with a template technique based on aromatic π-π-stacking interactions.

1994 Chengzhi Liang and Kurt Mislow find knotted proteins in a survey of structures deposited in the Brookhaven Protein Data Bank (PDB). Disulfide linkages are involved in forming the knot.

1995 Sigeo Ihara and Satoshi Itoh discuss the possible existence and the properties of toroidal single-walled carbon nanotubes. Experimentally, helical carbon nanotubes have been observed.

2000 Discovery of a protein with a deeply located knot, formed by the protein backbone itself (without participation of of disulfide bridges), in a survey of the PDB. Experimental discovery of a bacteriophage capsid which is formed by catenated proteins.

List of references for the lecture series on
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Books on Knots and Links

Textbooks, knot books, easy reading books, ...
— ordered alphabetically by the name of the (first) author (version of 9. September 2005)

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List of references for the lecture series on
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... roughly in chronological order ... (version of 9. September 2005)

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