Quantization of energy and writhe in self-repelling knots

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\textit{New Journal of Physics 4} (2002) 20.1–20.11 (http://www.njp.org/)

Received 19 December 2001, in final form 27 February 2002

Published 28 March 2002

\textbf{Abstract}. Probably the most natural energy functional to be considered for knotted strings is that given by electrostatic repulsion. In the absence of counter-charges, a charged, knotted string evolving along the energy gradient of electrostatic repulsion would progressively tighten its knotted domain into a point on a perfectly circular string. However, in the presence of charge screening self-repelling knotted strings can be stabilized. It is known that energy functionals in which repulsive forces between repelling charges grow inversely proportionally to the third or higher power of their relative distance stabilize self-repelling knots. Especially interesting is the case of the third power since the repulsive energy becomes scale invariant and does not change upon Möbius transformations (reflections in spheres) of knotted trajectories. We observe here that knots minimizing their repulsive Möbius energy show quantization of the energy and writhe (measure of chirality) within several tested families of knots.

1. Introduction

Knot theory was given a strong impetus when in the 1860s Kelvin proposed that knots made out of vortex lines of ether constitute elementary particles of matter, which at this time were thought to be atoms [1]. However, the development of atomic physics, first with classical and then with quantum models of atoms, failed to show a connection between knots and atoms. More recently though, today’s elementary particles are again considered to be stringlike objects that may be closed [2, 3] and perhaps knotted. This string theory approach partially revives the ideas
of Kelvin and provides a motivation for exploring quantization of energy and of other values in such physical systems such as knotted magnetic flux lines [4, 5] or knotted solitons [6].

Knots made of self-repelling, infinitely thin strings in three-dimensional Euclidean space have been considered by many authors [7]–[12]. Usually it was assumed that knots were perfectly flexible for bending but not extensible. The repelling charge was assumed to be continually spread along the knots so that there were no elementary point charges and that the charge contained within a given curvilinear segment was proportional to the length of this segment. When the Coulomb energy governed the evolution of a knot of this type one should observe that the knotted domain was progressively tightened into a singular point while the rest of the knot would form a perfect circle. Progressive tightening of knotted domains in electrostatic knots may seem counterintuitive when one considers that the electrostatic repulsion grows inversely proportionally to the square of the distance between every pair of charges. However, at the same time as tightening progresses, the length of the knotted domain decreases and therefore there is less and less charge in the tightly knotted domain. In fact the decrease of charge in the knotted domain is more rapid than its contribution to overall repulsion. Therefore the tightening that is driven by the decrease of the repulsion outside the knotted domain can progress until a knotted domain shrinks to a singular point and the entire string is perfectly circular. For this reason the Coulomb energy is not interesting as an energy functional for knots [13, 14]. However, it has been demonstrated that if the repulsion force were growing inversely proportionally to the third or higher power of the distance between the repelling elements, then the knotted domains in prime knots would have no tendency to shrink to a singular point [7, 8, 10, 12]. The third-power case is especially interesting from mathematical and physical points of view since the energy of a knot becomes conformally invariant and therefore does not change when the trajectory of the knot is rescaled or undergoes a Möbius transformation (reflection in a sphere) [10, 14, 15]. In this work we study configurations of knots that minimize their Möbius repulsive energy. From now on we will call these configurations Möbius knots. Several earlier studies used numerical simulations or an analytical approach to investigate various properties of Möbius knots [9, 15]; however, the relations between such characteristic properties of Möbius knots as their energy, crossing number, writhe or average crossing number (ACN) have not been systematically examined before.

2. Energy of Möbius knots

Let us consider first an unknotted closed string that has a few repulsive point charges equally separated and that the repulsion force between these charges grows inversely proportionally to the third power of their relative distance (such a repulsion behaviour is one of the necessary requirements to observe Möbius invariance). An energy-minimizing shape of such an unknotted highly flexible string would then be an equilateral polygon with the number of vertices (and edges) corresponding to the number of point charges. For example, if the string has three point charges the minimizing shape is an equilateral triangle, and in the case of four charges the minimizing shape is a square. To be able to operate with a model of a self-repulsive knot whose shape is independent of the number of charges in the knot one needs to assume that charges are not localized but continuously spread over the knot. This mathematical operation ensures that unknotted energy-minimizing strings would always form a perfect circle independently of the level of carried charge. However, this non-physical assumption of continuous charge redistribution causes the energy of a knot to become infinite due to the repulsion of nearby elements. In order to correct for this problem of infinite energies O’Hara [8] introduced a
regularization term and defined the energy
\[ \tilde{E}(K) = \iint_{K \times K} \left( \frac{1}{|x - y|^2} - \frac{1}{d_K(x, y)^2} \right) \, ds_K(x) \, ds_K(y) \]  
(1)
where \( d_K(x, y) \) is the shorter arc-length distance within \( K \) from \( x \) to \( y \). Notice that the integral of the second term corresponds to the repulsive energy of a straight segment with the same length and carrying the same charge as \( K \). Another, computationally more stable, approach is to neglect tangential contributions to repulsion as nearest-neighbour regions in smooth trajectories are practically collinear and define the cosine energy
\[ E(K) = \iint_{K \times K} \frac{1 - \cos \alpha}{|x - y|^2} \, ds_K(x) \, ds_K(y) \]  
(2)
where \( \alpha \) is the conformal angle between the tangents at points \( x \) and \( y \). In fact it was demonstrated by Doyle and Schramm (see [15]) that \[ \tilde{E}(K) = E(K) + 4. \]  
(3)
We have applied here the second approach and used Kenneth Brakke’s program Evolver to obtain Möbius-energy-minimizing configurations of various knots and to calculate their energies (see [16], also http://www.susqu.edu/facstaff/b/brakke/). Examples of configurations of various knots minimizing their Möbius energy can be seen in [15]. It should be recalled that actual shapes of Möbius energy minimizers of a given knot can substantially vary because all configurations obtained by Möbius transformations from one Möbius energy minimizer are also Möbius energy minimizers. In practice these shapes depend on an arbitrary choice of starting configurations used for the energy descent. However, the actual energy values obtained in our simulations converge to the same values independently of the starting configurations of a given knot. In addition we have checked that the values obtained by us for ten different \((2, p)\) torus knots were at most different by 0.1% from the values calculated using an analytical approach that can be applied to this class of knots [9, 15].

Figure 1 shows the relation between the Möbius energy and the topological, minimal crossing number for knots belonging to six different families of knots. We have analysed torus knots with Alexander–Briggs notation \( 3_1, 5_1, 7_1 \) etc, twist knots with even numbers of crossings (Alexander–Briggs notation \( 4_1, 6_1, 8_1 \) etc), twist knots with odd numbers of crossings (Alexander–Briggs notation \( 3_1, 5_2, 7_2, 9_2 \) etc) and three Conway families of knots with sign-independent Conway notations \((2p + 1, 1, 2p), (2p - 1, 2, 2p)\) and \((1, 2p - 1, 1, 2p - 1)\), where \( p \) are consecutive natural numbers (see figure 1(b) for a schematic explanation of how these families are formed). Standard representations of these knots classified according to Alexander–Briggs notations can be seen in tables of knots [17, 18] while the Möbius-energy-minimizing configurations are shown in [15] and one representative example of the energy-minimizing configurations of torus knot \( 11_1 \) is shown here in figure 1(c). From the data points in figure 1(a) we have excluded founders of the families as these frequently belong to different families at the same time. It is visible that in all these knot families the energy grows with practically identical rates, that seem to be linear. A linear fit over the tested range indicates that for each new crossing the energy grows by around 26–27 units. To give an estimation of energy units it is good to point out here that within the energy defined by the equation (1) the energetic cost of closing an open string into an unknotted circle is exactly 4 units [14]. Notice that some of the plotted lines in figure 1(a) practically coincide with each other, while others seem to be vertically shifted by a constant value.

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Figure 1. Energy of Möbius knots. (a) Different families of torus knots, twist knots and Conway knots show the same slope. These analysed families are represented in (b) with $k = 1$ and $p = 2$ (we adopted here a sign-independent notation). (c) The difference of energy between sequential torus knots tends asymptotically towards 52.8, which corresponds to 26.4 for each new crossing. The inset shows one of the configurations of the torus knot $11_1$ that minimizes the Möbius repulsive energy; its position on the plot is indicated. Notice that the actual dimensions of the knot shown are not relevant as the shape of the energy minimizer is independent of scale.

A closer look at energy values for the $(2, p)$ torus knot family ($3_1, 5_1, 7_1$ etc), including the founder $3_1$ knot, suggests that the energy difference between consecutive torus knots shows an asymptotic convergence toward a constant value of nearly 53. Since the energy minimization by simulation with Evolver (or other programs) has its well known limitations in descending toward a global minimum, especially for complex trajectories, we have used an analytical approach to generate torus knots configurations that are believed to be minimizers of the Möbius energy [9, 15]. Figure 1(c) shows that the difference of energy between sequential torus knots tends asymptotically toward 52.8, which corresponds to 26.4 for each new crossing.
On the basis of our simulation data (figure 1(a)) and analytical approach (figure 1(c)) we conjecture that within such families of knots that iteratively increase their interwound regions with double-helix structure [15] the differences in Möbius energy due to each new crossing tend to an universal constant value.

3. Writhe of Möbius knots

As already discussed, knots minimizing Möbius energy do not have unique shapes since Möbius transformations can create infinitely many different configurations that minimize the Möbius energy for a given knot. However, certain characteristic properties of curves in space are constant upon change of the scale and other forms of Möbius transformation. It was proven by Banchoff and White that the absolute value of writhe for a given trajectory is invariant upon Möbius transformation [19]. Writhe (Wr) measures the extent of chirality of closed curves in space and therefore provides an interesting measure for knotted trajectories minimizing a given energy functional. The writhe corresponds to the average signed number of perceived self-crossings when an oriented closed curve is observed from a random point on a sphere enclosing a given trajectory and where each right-handed crossing is scored as +1 and each left-handed crossing is scored as −1. The value of writhe (Wr) is usually calculated using the Gauss integral formula

$$\text{Wr} = \int \int_{K \times K} \frac{(u \times v) \cdot (x - y)}{|x - y|^3} \, ds_K(x) \, ds_K(y) \tag{4}$$

where $u$ and $v$ are the unit tangent vectors to $K$ at $x$ and $y$, respectively. In the case of tight knots minimizing their rope length and that are known as ideal, the writhe values showed a quantization [20]–[22] and the quantum of writhe depended on the type of crossing introduced [23, 24]. We decided therefore to check whether knots minimizing their Möbius energy also show a similar quantization of writhe.

Figure 2(a) illustrates that torus and twist families of Möbius knots show a clear quantization of writhe, where the writhe increase for torus knots is more rapid than for twist knots. While the differences of energy within a given family were showing an asymptotic descent toward a limiting constant value (figure 1(c)), the differences of writhe showed a specific constant value (within the accuracy of our computational approach) that seemed to be independent of the complexity of the knot. In the case of ideal knots (see figure 2(b)) it was observed earlier that the slopes of writhe increase for torus knots and twist knots were described by simple relations: $1 + x$ and $1 - x$ respectively [23, 24], where $x$ was the same for both families and seemed to correspond to three-sevenths [25, 26] and where the integer value 1 (or −1 depending on the handedness of crossing) is due to the inter-coil crossing contribution while the noninteger value $x$ is due to the intra-coil contribution to writhe [23]. We observed here that the slopes of writhe increase for Möbius torus and twist knots also show opposing deflections from the slope of unity; however, the deflection value $x$ is close to one-fifth instead of three-sevenths. Thus torus-type turns with positive signs of crossings introduce a writhe of around 1.2 per crossing. Twist-type turns with positive signs of crossings introduce a writhe of about 0.8 per crossing. Torus- and twist-type turns can be recognized by the orientation along both arcs enclosing double-arc fields in minimal crossing diagrams of a knot [23]. Parallel and anti-parallel orientations characterize torus- and twist-type turns, respectively [23].

In the case of ideal knots it was observed that the writhe of achiral knots was essentially equal to zero [20, 24]. We observed here the same tendency for knots minimizing their Möbius energy,
Figure 2. Writhe of Möbius knots. (a), (b) The quantization of absolute writhe of Möbius knots and ideal knots, respectively; the analysed families are torus knots and twist knots. (c) Absolute writhe slopes for all families of knots tested by us. Notice the constant increase of writhe within each analysed family of Möbius knots.

as all achiral knots tested by us (i.e. 4₁, 6₃, 8₃, 8₀, 8₁₂, 8₁₇ and 8₁₈) had their writhe practically equal to zero.

Figure 2(c) shows absolute writhe slopes for all families of knots tested by us. It is visible that within each of these families of knots there is an apparently constant, specific increase of writhe as one analyses consecutive members of respective families. Interestingly the increase of writhe can be simply predicted by analysing the type of turn that is introduced when creating the next member of a family, so for example in the −(2p+1, 1, 2p) Conway family, as one goes from a knot to its successor four new crossings are introduced: two are positive torus crossings, which increase the writhe by about 2.4, and two are negative twist crossings, which decrease the writhe by about 1.6. Therefore the predicted increase of writhe of about 0.8 when divided by four crossings gives us the observed slope of about 0.2 (see figure 2(b)). We can similarly predict and explain why knots from even and odd twist families of knots follow slopes with the
Figure 3. Odd and even twist knots differ in the sign and type of crossing in the terminal clasp. Odd twist knots have terminal clasps with torus-type crossings (orientations along the arcs enclosing this double-arc field are parallel), while even twist knots have twist-type crossings (orientations along the arcs enclosing this double-arc field are anti-parallel). Notice that the sign of crossings in the terminal clasp also changes, although signs and types of crossings in the interwound region remain the same.

same inclination but that are vertically shifted by exactly four units in relation to each other. Figure 3 shows that change from an odd to an even twist family of knots implies that two torus-type crossings in the terminal clasp are replaced by two twist-type crossings of opposite sign. Since the corresponding writhe contributions of these crossings are \(1 + x\) and \(-1 + x\) (or \(-1 - x\) and \(1 - x\) for opposite handedness), where \(x\) is a constant, the resulting absolute difference of writhe is two per crossing regardless of the actual value of intra-turn contribution \((x)\) to writhe. Since there is a change of two crossings, the global difference of writhe between even and odd twist families of knots results in the observed vertical shift of corresponding writhe slopes by exactly four. We can apply a very similar type of reasoning to explain why Conway families \((2p + 1, 1, 2p)\) and \((2p - 1, 1, 2p)\) differ in their corresponding values of writhe by exactly two. Notice that the same type of explanation (where intra-turn contributions to writhe cancel) applies not only to Möbius knots but also to ideal knots. Figure 2(b) shows that in the case of ideal knots, odd and even twist families of knots results in the observed vertical shift of corresponding.writhe slopes by exactly four. Axial trajectories of ideal knots (rope length minimizing) can be regarded as a limit of energy-minimizing configurations when the energy is taken to be an integral of an ever-increasing inverse power of the radius of certain circles passing through three points of the curve [25]. Therefore this observation strongly suggest that minimizers of repulsive functionals with any exponent between 3 and \(\infty\) will always have a constant shift of writhe slopes between certain families of knots. Thus for example slopes of absolute writhe for even and odd twist knots will always show a relative vertical shift by exactly four (compare figures 2(a) and (b)) provided that compared knots minimize the same repulsive functional with the exponent ranging between 3 and \(\infty\).

4. Relations between energy and crossings

There are two principal measures of crossings applied to knots. Minimal crossing number is a topological invariant and corresponds to the minimal number of crossings that any representation of this knot type can have in any orthogonal projection. ACN applies to a given rigid embedding of a knot and corresponds to the average number of perceived crossings (irrespective of their
Figure 4. Relation between the energy and crossings for all prime knots up to nine crossings. (a) The relation between Möbius energy and minimal crossing number for all prime knots up to nine crossings. The upper and lower bounds were best fits of power law functions $y = ax^n$. Fits satisfied the condition that no experimental point was outside the bounds. (b) The relation between Möbius energy and ACN for all prime knots up to nine crossings. (c) The energy as a function of ACN within different families of knots.

handedness) when this particular embedding is perceived from a random point on a sphere enclosing a given trajectory. The ACN value can be calculated using the unsigned Gauss integral formula

$$\text{ACN} = \int \int_{K \times K} \frac{|(u \times v) \cdot (x - y)|}{|x - y|^3} \, ds_K(x) \, ds_K(y)$$

where $u$ and $v$ are the unit tangent vectors to $K$ at $x$ and $y$, respectively. Notice the similarity in the definitions of writhe and ACN; indeed, we obtain ACN from Wr by replacing the integrand by its absolute value. Several studies considered theoretically the relation between the Möbius invariant repulsive energy and the two measures of crossings mentioned above. Freedman et al [10] demonstrated for example that the Möbius energy of a knot is at least $2\pi$-fold bigger than the minimal crossing number of this knot. Figure 4(a) shows the relation between Möbius

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energy and minimal crossing number of all knots up to nine crossings. It is visible that data points fill a ‘cone’ and that for these relatively simple prime knots the lower linear bound of the energy could be put at least at \(7.47\pi\) times the minimal crossing number. One can also analyse the upper bound for the energy as a function of minimal crossing number. In figure 1(a) we have shown that within a given family the energy grows proportional to the crossing number, but as the crossing number increases, founders of new families arise and these can have very high energy as compared with the members of already established families. Thus for example a twist knot \(8_1\) has the energy of 217 while the \(8_{18}\) knot founding a new family has the energy of 284. The upper bound of the energy does not follow a linear relation with the crossing number but approaches a \(7/5\) power law (see figure 4(a)).

The ACN value is not invariant upon Möbius transformation; however, we have checked that ACN value is very robust and hardly changes upon multiple Möbius transformations. Therefore it seems reasonable to investigate the relation between the energy and ACN of Möbius knots. Freedman et al [10] showed that the Möbius energy of a knot increased by \(56/11\) is at least \(12\pi/11\) times bigger than the ACN of energy-minimizing configurations. The existence of this linear lower bound demonstrates that the Möbius energy cannot grow with a power lower than unity as a function of ACN. It could however grow with a higher power. In fact our own data (figure 4(b)) indicate that data points for the relation between the energy and ACN fill a much narrower ‘cone’ than was the case for the relation between the energy and minimal crossing number (see figure 4(a)). The lower bound of this cone can be described by a nearly linear function; this function is given by

\[
y = 22.25 \cdot x^{1.05}
\]

whereas the upper bound is better described by a nearly \(7/5\) power law,

\[
y = 14.78 \cdot x^{1.42}.
\]

This power law behaviour may seem inconsistent with a linear growth of energy with the ACN within different analysed families of knots (figure 4(c)). However as the ACN increases, new founders for each family of knots enter, and they frequently start their families with a linear growth but at a higher level. Again \(8_1\) and \(8_{18}\) knots are good examples as the difference of their energy is much bigger than expected from a slightly higher ACN of \(8_{18}\) knot.

5. Möbius knots and their relation to random knots and other knotted physical systems

It was shown earlier that the average writhe for a population of random knots of a given type closely corresponds to the writhe of a tight or ideal (rope-length-minimizing) knot of the corresponding type [20, 26]. We have shown here that with the exception of achiral knots the writhe values of Möbius knots do not correspond to those of ideal knots. Although within given families there is a linear relation between writhe of ideal and Möbius knots these relations are not universal and different families will be related by different linear relations. Thus for example the writhe of torus knots grows more quickly for ideal knots than for Möbius knots but the opposite is true for twist knots. Therefore we can conclude here that the writhe of Möbius knots is not related to the writhe of random knots of corresponding type.

The time-averaged writhe value of randomly fluctuating knots of a given type seems to be independent of the length of random chains forming a given knot. This is not the case for ACN, as...
its value progressively increases with the length of a random chain. However, it was observed that for relatively simple knots the differences between time-averaged ACNs of randomly fluctuating knots of a given type and of unknots of the same chain size closely correspond to the ACN of ideal knots of the corresponding types [14]. However this does not apply to ACN values of Möbius knots since these are significantly smaller than ACN values of corresponding ideal knots. We conclude therefore that Möbius knots in contrast to ideal knots are not good predictors of certain physical properties of random knots of a given type such as knotted polymer molecules undergoing a random thermal motion. However for other physical knotted systems, Möbius knots may better approximate their behaviour than ideal knots. If we imagine a charged knotted string of dimensions comparable to an effective screening radius at given conditions, then all pairwise interactions within such a knot should be repulsive. However, due to screening interactions caused by counterions the repulsion would not follow the Coulomb law but would decrease more rapidly with the separating distance, approaching perhaps an inverse cubic dependence of the distance. Short flexible polymeric molecules such as single-stranded DNA can make knots of dimensions comparable to the effective screening radius at specific ionic conditions, and such knots may then approximate the Möbius behaviour. In fact, one might attempt to observe such DNA knots spontaneously undergoing Möbius transformations of shape when driven by very small thermal fluctuations, as has been seen for phospholipid vesicles [27]. Finally, one can entertain a thought about stringlike charged elementary particles (electrons, for example) surrounded by a short-lived mixture of other charged particles and antiparticles generated from quantum fluctuation of the vacuum. Electrons may then minimize an energy that resembles the Möbius energy described here. If on the way to relaxation a complex self-repelling knot could undergo from time to time a strand passage and progressively simplify its type, that would provide a physical system with natural quantization of the energy.

Acknowledgments

We thank François Ubertini and Akos Dobay for their help in solving frequent software and hardware problems, Piotr Pieranski and Corinne Cerf for discussions on writhe quantization, Jun O’Hara and John Maddocks for discussions on energy of knots and Jacques Dubochet for his keen interest and constant encouragement. We also thank Kenneth Brakke for making available his program Evolver. This work was supported by Swiss National Science Foundation grant 31-61636.00 to AS and by United States National Science Foundation grant DMS 00-76085 to RK.

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