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A simple energy function for knots

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Abstract

An energy function is defined for C^2 knots. It is shown that the function has several attractive qualities: it is scale invariant; it "blows up" if the knot is self-intersecting (so that on the energy hypersurface knot types are separated by infinitely high potential walls); it has a relatively simple definition and a pseudo-physical interpretation.

Keywords: Knot; Energy; Energy of a knot; Complexity of a knot

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1. Introduction

Recently there has been an increased interest in what might be termed physical knot theory. The general procedure is to define a function, thought of as energy, on some class of knots. One hopes to learn something about knot-types by studying the energy surface. The papers [4,5,7,11] all consider the class of piecewise linear knots. [2,3,6,8–10] consider the smooth case. Most of this work has been amenable to computer simulation.

Usually a knot K is defined as an embedding of the circle into $\mathbb{R}^3$. We will call an immersion of the circle that is not an embedding a self-intersecting knot. Speaking loosely, we will use the term knot for self-intersecting knots as well.

Let $E(K)$ be our energy function. In the work mentioned above it is assumed that $E(K)$ ought to have the following attributes:

(1) $E(K)=\infty$ if K is self-intersecting,

(2) $0<E(K)<\infty$ if K is not self-intersecting.

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Together these attributes ensure that we can associate an energy surface with the knots and that on this surface knot-types are separated by infinitely high potential walls. We can also say that the critical points of the energy surface are special conformations of the knots. For example, we might say that a global minimum for a knot-type is a canonical conformation for that knot-type. In general, any description of the energy surface for a knot-type is also an invariant.

In this paper we introduce a new potential energy function for smooth knots. This function has several attractive properties: it is defined as a simple double integral, it is scale invariant, it has attributes (1) and (2) above, and it has a sensible pseudo-physical interpretation. From the definition of the energy we expect that the "more complicated" the knot the greater its potential energy at its minimum conformation. Our main results are the definition of the energy function, $E(K)$ and the proof that it has attributes (1) and (2) above.

2. Definition of $E(K)$

A C^2 knot is an embedding of S^1 in $\mathbb{R}^3$ that is twice continuously differentiable. Let K and L be C^2 knots. Note that at each point $x \in K$ there is a unique plane normal to K. We will denote this plane by N_x. Define $\mathrm{Proj}_{N_x}(v)$ to be the projection of v onto N_x.

We define $E(K, L)$ as:

$$E(K, L) = \int_{y \in L} \int_{x \in K} \left| \mathrm{Proj}_{N_x}\left(\frac{y - x}{|y - x|^2} \right) \right|^2 \mathrm{d}x \, \mathrm{d}y \tag{2.1}$$

where $\mathrm{d}x$ and $\mathrm{d}y$ are the differentials of arc length.

In order to extend this definition to knots with self-intersections we have to deal with the nonuniqueness of the normal plane at intersection points. Fortunately this is not difficult: let $\alpha : [a, b] \to \mathbb{R}^3$ and $\beta : [c, d] \to \mathbb{R}^3$ be two C^2 curves parametrized by arc length. For any vector v we let N_v be the plane with normal vector v. We define $E(\alpha, \beta)$ as:

$$E(\alpha, \beta) = \int_c^d \int_a^b \left| \mathrm{Proj}_{N_{\alpha'(t)}}\left(\frac{\beta(s) - \alpha(t)}{|\beta(s) - \alpha(t)|^2} \right) \right|^2 \mathrm{d}t \, \mathrm{d}s.$$

If α and β are parametrizations of the knots K and L then the two definitions of energy agree. The second definition makes sense whether or not the curves have self-intersection. Therefore if the knots K and L have self-intersections we can compute $E(K, L)$ by choosing parametrizations and using the second definition of the energy.

Now, for any knot K we define $E(K) = E(K, K)$. Notice that $E(K)$ is scale invariant. That is, for any $r > 0$ we have $E(rK) = E(K)$.

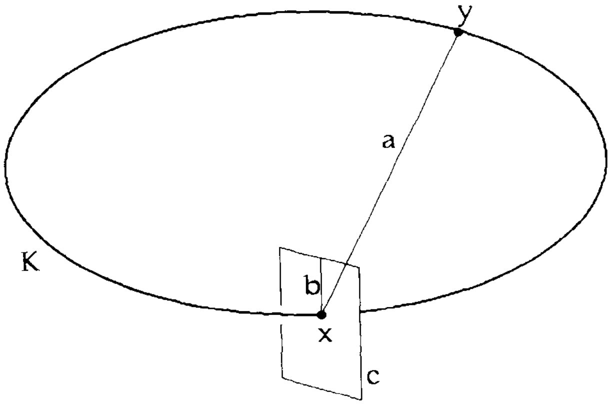

Fig. 1. $a = |y-x|$, $b = \mathrm{Proj}_{N_x}((y-x)/|y-x|^2)$, $c = N_x$.

As a pseudo-physical interpretation we note that the energy is given by integrating the power of an inverse distance, except we are interested only in the normal component of this inverse distance (see Fig. 1).

3. Proof that $E(K)$ has attribute (1)

Let $\gamma(t)$ be a C^2 parametrization (by arc length) of the knot K. Since K has self-intersections, we can assume that there is a point p on K, a number δ and two C^2 parametrizations (by arc length), α and β, of K such that:

(1) $\alpha(0) = \beta(0) = p$,

(2) $\alpha(t) = \beta(s)$ for $0 \leqslant s,t \leqslant \delta$ only if $s = t = 0$,

(3) $\alpha'(0) \cdot \beta'(0) \geqslant 0$. (The angle between the vectors is $\leqslant \pi/2$.)

We divide the proof into two cases: tangential intersections and transverse intersections.

3.1. *Tangential intersections*

Here we assume that $\alpha'(0) = \beta'(0)$. The proof requires a series of elementary calculus lemmas. Since the technical details might obscure it, we start by describing the basic idea behind the proof. If γ_1 and γ_2 are straight-line segments on opposite sides of a square then $E(\gamma_1, \gamma_2) = c$ (the precise value of c is unimportant). The scale invariance of the energy function tells us that c is independent of the size of the square. Our idea is to divide one branch of the knot (from the intersection point) into an infinite number of segments. We then pair each of these segments with one on the other branch so that they are approximately the opposite sides of a square. Therefore the energy of each of these pairs is bounded below. Summing the contribution of all the pairs of segments gives infinity, which proves attribute (1).

For the following four lemmas we will assume that $\gamma:[0, d] \to \mathbb{R}^3$ is a C^2 curve parametrized by arc length. We fix a number M such that the curvature of γ is everywhere less than M, that is $|\gamma''(t)| < M$ for all $0 \leqslant t \leqslant d$. The proofs of these lemmas are all elementary. We include them because they are quite brief and doing so might save the reader some grief.

The first lemma gives a bound on how fast the tangent vector can turn.

Lemma 3.1. *If* $1 - Md > 0$ *then* $\gamma(s) \cdot \gamma'(t) \geqslant 1 - Md$ *for all* $s,t \in [0, d]$.

Proof. We can assume that $s < t$. Thus

$$\gamma'(s) \cdot \gamma'(t) = \int_s^t \gamma'(s) \cdot \gamma''(u)\, \mathrm{d}u + \gamma'(s) \cdot \gamma'(s).$$

Since $|\gamma'(s)| = 1$ and $|\gamma''(t)| < M$ the right-hand side is greater than $1 - M(t - s) \geqslant 1 - Md$. $\square$

Our next lemma gives bounds on how well γ approximates a straight line.

Lemma 3.2. *Let* $\gamma'(0) = v_1, v_2, v_3$ *be an orthonormal basis of* $\mathbb{R}^3$. *If* $1 - Md > 0$ *the curve* $\gamma([0, d])$ *is contained in the cylinder*

$$\left\{\gamma(0) + tv_1 + bv_2 + cv_3 \,|\, 0 \leqslant t \leqslant d \text{ and } b^2 + c^2 \leqslant \frac{M^2d^4}{2}\right\}.$$

(*See Fig*. 2.)

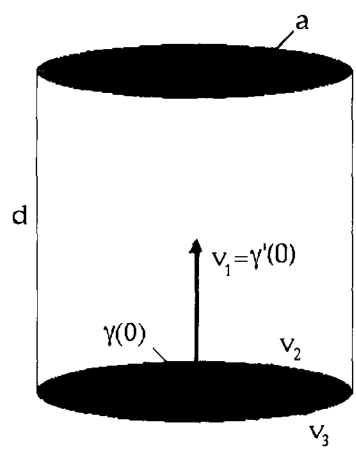

Fig. 2. $a = \frac{1}{2}\sqrt{2}Md^2$.

Proof. We can write $\gamma(t)=\Sigma_i a_i(t)v_i$. Thus

$$\begin{aligned}\gamma(t)&=\gamma(0)+\int_0^t\gamma'(s)\,\mathrm{d}s\\&=\gamma(0)+\int_0^t a_1'(s)v_1\,\mathrm{d}s+\int_0^t\left(\int_0^s a_2''(u)\,\mathrm{d}u+a_2'(0)\right)v_2\,\mathrm{d}s\\&\quad+\int_0^t\left(\int_0^s a_3''(u)\,\mathrm{d}u+a_3'(0)\right)v_3\,\mathrm{d}s.\end{aligned}$$

Now $a_2'(0)=a_3'(0)=0$. Thus,

$$\gamma(t)=\gamma(0)+\int_0^t a_1'(s)v_1\,\mathrm{d}s+\int_0^t\int_0^s a_2''(u)\,\mathrm{d}u\,\mathrm{d}s\cdot v_2+\int_0^t\int_0^s a_3''(u)\,\mathrm{d}u\,\mathrm{d}s\cdot v_3.$$

Since $a_1'(0)=1$ and $|a_1'(s)|<M$ we get $1-Mt\leqslant a_1'(s)\leqslant 1$. This implies $0\leqslant\int_0^t a_1'(s)\,\mathrm{d}s\leqslant t'\leqslant d$. For $j=2, 3$ we know $|a_j''(s)|<M$. This implies

$$\left|\int_0^t\int_0^s a_j''(u)\,\mathrm{d}u\,\mathrm{d}s\right|\leqslant\frac{Mt^2}{2}\leqslant\frac{Md^2}{2}.$$

This proves the lemma. □

We will describe the cylinder in Lemma 3.2 as the cylinder based at $\gamma(0)$ of length d and radius $\frac{1}{2}\sqrt{2}Md^2$ with axis $\gamma'(0)$. (See Fig. 2.)

Corollary 3.3. *Suppose w is a unit vector, such that $w\cdot\gamma(0)=r\geqslant Md$. Then $\gamma([0, d])$ is contained in the cylinder based at $\gamma(0)$ of length d and radius $\sqrt{2}\,(\frac{1}{2}Md^2+d\sqrt{1-r^2})$ and axis w.*

Proof. The proof is the same as that of Lemma 3.2: use an orthonormal basis $w=v_1, v_2, v_3$ and keep in mind that $a_2'(0)$ and $a_3'(0)$ are not 0 but are less than $\sqrt{1-r^2}$. □

Lemma 3.4. *There is a positive number $R\leqslant 1$ such that if v and w are unit vectors with $v\cdot w\geqslant R$ and x is any vector with $|\mathrm{Proj}_{N_w}(x)|\geqslant\frac{1}{5}\sqrt{5}\,|x|$ then $|\mathrm{Proj}_{N_v}(x)|\geqslant\frac{1}{4}|x|$. (Recall N_w is the plane with normal w.)*

Proof. The proof is a triviality. The lemma simply states that if the angle between v and w is small enough and the angle between x and w is bigger than $\arctan(\frac{1}{5}\sqrt{5})$ then the angle between v and x is greater than $\arctan(\frac{1}{4})$. □

The following lemma is the technical statement of our insight that if two curves are approximately the opposite sides of a square then the potential energy between them is bounded below by a positive number.

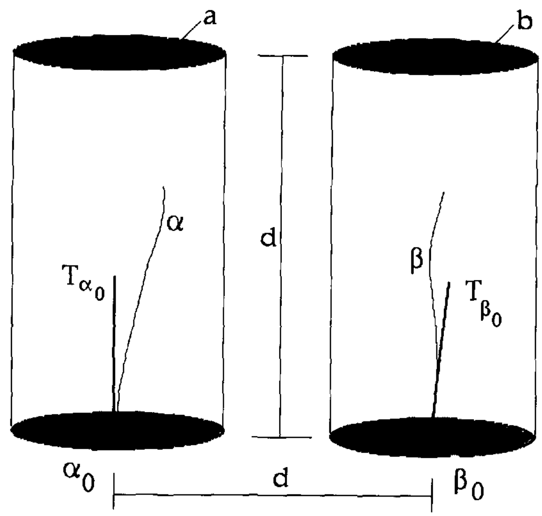

Fig. 3. $a=\frac{1}{2}\sqrt{2}Md^2$, $b=\sqrt{2}(\frac{1}{2}Md^2+d\sqrt{1-r^2})$.

Lemma 3.5. *Suppose α and β are C^2 curves of total arc length d. Let α_0 and β_0 be their initial points and let T_{α_0} and T_{β_0} be their initial unit tangent directions. Let R be the number from Lemma 3.4. We assume there are numbers M and r such that:*

(1) *The curvatures of α and β are bounded by M.*
(2) (a) $1-Md>r>Md$, (b) $r>R$, (c) $1-\sqrt{2}Md-\sqrt{2}\sqrt{1-r^2}>\frac{1}{2}$.
(3) $T_{\alpha_0}\cdot T_{\beta_0}>r$.
(4) $T_{\alpha_0}\cdot(\beta_0-\alpha_0)=0$.
(5) $|\beta_0-\alpha_0|=d$.

Given the above assumptions $E(\alpha,\beta)>1/3000$.

Proof. There is no harm in assuming that $\alpha,\beta:[0,d]\to\mathbb{R}^3$ and C^2 curves parametrized by arc length. By Lemma 3.2 the curve $\alpha([0,d])$ is contained in the cylinder based at $\alpha(0)$ of length d and radius $r_1=\frac{1}{2}\sqrt{2}Md^2$ with axis $\alpha'(0)$. Likewise, by Corollary 3.3 and assumptions (2a) and (3) the curve $\beta([0,d])$ is contained in the cylinder based at $\beta(0)$ of length d and radius $r_2=\sqrt{2}(\frac{1}{2}Md^2+d\sqrt{1-r^2})$ with axis $\alpha'(0)$. (See Fig. 3.) By considering these two cylinders we see that $|\beta(s)-\alpha(t)|^2\leqslant d^2+(d+r_1+r_2)^2\leqslant\frac{13}{4}d^2$. The last inequality follows from assumption (2c). Similarly we see that

$$|\beta(s)-\alpha(t)|\geqslant d-r_1-r_2\geqslant\frac{d}{2}. \tag{3.1}$$

We also see that

$$\begin{aligned}|\mathrm{Proj}_{N_{\alpha'(0)}}(\beta(s)-\alpha(t))| &\geqslant\frac{d-r_1-r_2}{\sqrt{d^2+(d-r_1-r_2)^2}}|\beta(s)-\alpha(t)|\\ &\geqslant\frac{1}{\sqrt{5}}|\beta(s)-\alpha(t)|.\end{aligned}$$

The last inequality follows from equation (3.1).

Now by Lemma 3.1 and assumption (2a) we have $\alpha'(0)\cdot\alpha'(t)\geqslant 1-Md\geqslant r$. Thus by Lemma 3.4 and assumption (2b) we have

$$|\mathrm{Proj}_{N_{\alpha(t)}}(\beta(s)-\alpha(t))|\geqslant\tfrac{1}{4}|\beta(s)-\alpha(t)|\geqslant\frac{d}{8}.$$

Thus

$$E(\alpha,\beta)=\int_0^d\int_0^d\frac{|\mathrm{Proj}_{N_{\alpha(t)}}(\beta(s)-\alpha(t))|^2}{|\beta(s)-\alpha(t)|^4}\,\mathrm{d}s\,\mathrm{d}t\geqslant\int_0^d\int_0^d\frac{d^2/64}{(13/4)^2d^4}\,\mathrm{d}s\,\mathrm{d}t$$
$$\geqslant\tfrac{1}{3000}.$$

This proves the lemma. □

We can now proceed with the proof that the energy function has attribute (1). Recall our assumptions for α and β:

(1) α and β are C^2 parametrizations by arc length of K.
(2) $\alpha(0)=\beta(0)=p$, $\alpha'(0)=\beta'(0)$.
(3) For $0\leqslant s,\ t\leqslant\delta$, $\alpha(t)=\beta(s)$ if and only if $t=s=0$.

In addition we fix M such that $M\geqslant|\alpha''(t)|$ and $M\geqslant|\beta''(t)|$ for all $t\in[0,\delta]$.

Let $N(t)$ be the normal plane to α at $\alpha(t)$. Therefore the condition that $\beta(s)$ is on $N(t)$ is $\alpha'(t)\cdot(\beta(s)-\alpha(t))=0$. We will need to be assured of the existence of such points $b(s)$ with certain properties. For this we use the implicit function theorem. Define $f(t,s)=\alpha'(t)\cdot(\beta(s)-\alpha(t))$. We have:

(1) $$\frac{\partial f}{\partial s}(t,s)=\alpha'(t)\cdot\beta'(s),\qquad\frac{\partial f}{\partial s}(0,0)=1.$$

(2) $$\frac{\partial f}{\partial t}(t,s)=\alpha''(t)\cdot(\beta'(s)-\alpha(t))-1,\qquad\frac{\partial f}{\partial t}(0,0)=-1.$$

(3) $$f(0,0)=0.$$

Thus the implicit function theorem states that there are subintervals $[0,\delta_1]$ and $[0,\delta_2]$ of $[0,\delta]$ and a continuous increasing function $g:[0,\delta_1]\to[0,\delta_2]$ such that for all $(t,s)\in[0,\delta_1]\times[0,\delta_2]$ we have $f(t,s)=0$ if and only if $s=g(t)$. Note, $\beta(g(t))$ is the unique point in $\beta([0,\delta_2])$ on $N(t)$ (see Fig. 4).

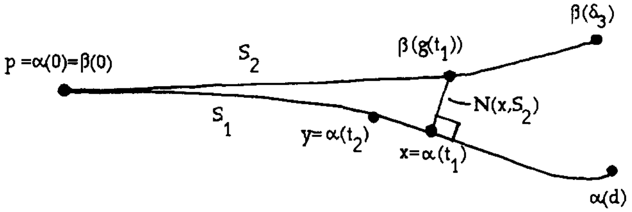

Fig. 4.

Fix $d < \delta_1$ small enough so that we can choose an r satisfying condition (2) of Lemma 3.5. Making d smaller if necessary choose $\delta_3 \leqslant \delta_2$ such that:

(1) $g : [0, d] \to [0, \delta_3]$,

(2) $\alpha'(t) \cdot \beta'(s) \geqslant r$ for all $t \in [0, d]$, $s \in [0, \delta_3]$.

We need a little more notation. Denote $\alpha([0, d])$ by S_1 and $\beta([0, \delta_3])$ by S_2. For x on S_1 define $N(x, S_2)$ to be the distance from x to the unique point of intersection between S_2 and the normal plane to S_1 at x. That is, if $x = \alpha(t)$ then $N(x, S_2) = |\alpha(t) - \beta(g(t))|$.

Finally, for $x, y \in S_1$ (S_2) define $d(x, y)$ to be the distance from x to y along S_1 (S_2). (If $x = \alpha(t_1)$ and $y = \alpha(t_2)$ then $d(x, y) = |t_2 - t_1|$.) (See Fig. 4.)

Since $N(\alpha(t), S_2)$ is continuous in t and $N(\alpha(0), S_2) = 0$ we can choose $t_1 \in (0, d]$ such that

$$\delta_3 - g(t) \geqslant N(\alpha(t), S_2) \quad \text{for all } 0 \leqslant t \leqslant t_1. \tag{3.2}$$

That is, if $q = g(\alpha(t)) \in S_2$ is the (unique) point on the normal plane to S_1 at $\alpha(t)$ then the distance from q to the end of S_2 is greater than the distance from $\alpha(t)$ to q.

We now construct a partition of S_1 into disjoint segments and pair each segment to one on S_2. Keep d, δ_3, and t_1 as constructed above.

Since the function $N(\alpha(t), S_2)$ is 0 when $t = 0$ and positive when $t = t_1$ there is a number $0 < t_2 < t_1$ such that $N(\alpha(t_2), S_2) = d(\alpha(t_2), \alpha(t_1))$. Proceeding recursively, choose $0 < t_{j+1} < t_j$ such that $N(\alpha(t_{j+1}), S_2) = d(\alpha(t_{j+1}), \alpha(t_j))$. Let $d_j = N(\alpha(t_{j+1}), S_2) = d(\alpha(t_{j+1}), \alpha(t_j))$. Also, let $s_j = g(t_j)$.

Define α_j to be the curve $\alpha([t_{j+1}, t_j])$. By the construction of t_1 (see equation (3.2)), we have $s_{j+1} + d_j < \delta_3$. Therefore the curve $\beta_j = \beta([s_{j+1}, s_{j+1} + d_j])$ is well defined and contained in S_2 (see Fig. 5).

Lemma 3.5 implies $E(\alpha_j, \beta_j) \geqslant 1/3000$ for each j. Since the curves α_j are mutually disjoint (except possibly at their endpoints) the double integral $E(K, K) \geqslant \Sigma_j E(\alpha_j, \beta_j) = \infty$. This proves E has property (1).

3.2. *Transverse intersections*

This case can be proved in a manner similar to the previous case. Another approach is to write (t, s) in polar coordinates $(r \cos \theta, r \sin \theta)$. It is easy to show

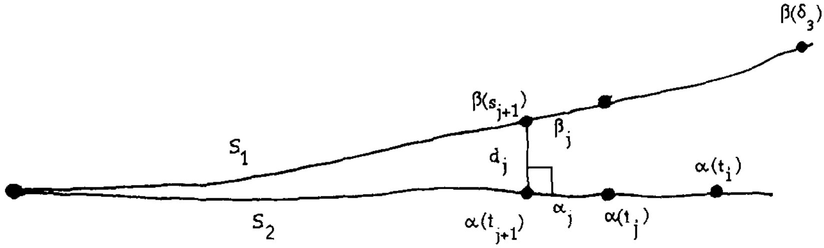

Fig. 5.

that for θ bounded away from 0 both $|\mathrm{Proj}_{N_{\alpha'(t)}}(\beta(s)-\alpha(t))|$ and $|\beta(s)-\alpha(t)|$ are of order r. So the integrand in the energy integral is of order r^{-2}. Hence, the energy is infinite.

4. Proof that $E(K)$ has attribute (2)

Suppose γ is a parametrization by arc length of K. Let M be its maximum curvature. For any t, s we have $|\gamma(t+s)-\gamma(t)-s\gamma'(t)| \leqslant \frac{1}{2}Ms^2$. Thus $|\mathrm{Proj}_{N_{\gamma(t)}}(\gamma(s+t)-\gamma(t))| \leqslant \frac{1}{2}Ms^2$. Similarly, for $|s| < 1/M$ we have $|\gamma(s+t)-\gamma(t)| \geqslant \frac{1}{2}s$. Thus, in a neighborhood of the diagonal $\{(x, x) | x \in K\}$ the integrand of the energy integral (2.1) is bounded. Since for curves without self-intersection outside of any neighborhood of the diagonal the integrand is bounded the energy integral must be finite. This proves that $E(K)$ has attribute (2).

5. Remarks

(1) We can compute directly that the energy of any circle is π^2.

(2) As mentioned in the introduction the energy at a minimum for a knot-type is an invariant for that knot-type. Moreover the position (modulo rigid motions and scaling) is also an invariant and might be called a canonical position. These invariants can be approximated using a computer. A routine which does this has been added to K. Brakke's Surface Evolver program (available from the Geometry Center at the University of Minnesota). Also, the authors have done some computations for an energy function developed for piecewise linear knots, see [4].

(3) A direct connection can be shown between this energy and the topological invariant crossing number. Specifically, let $c[\gamma]$ denote the crossing number of the curve γ. Then we have $E[\gamma] \geqslant 4\pi c[\gamma]$. We can say then, for example, that any curve with energy less than 12π is unknotted, since the trefoil requires three crossings. Some of these results parallel some of those proved in [2,6] for an energy introduced in [10].

(4) We can define another energy function for knots, with some but not all of the attractive properties of E, as follows: For $x \in K$ let $N(x, R)$ be the solid disk of radius R centered at x contained in the normal plane N_x. Define

$$R(K) = \max\{R \,|\, N(x, R) \cap N(y, R) = \emptyset \text{ for all } x, y \in K \text{ with } x \neq y\}.$$

Heuristically $R(K)$ can be thought of as the diameter of the thickest rope that can be used to tie the knot. We can define the energy function as $E^*(K) = 1/R(K)$. Attributes (1) and (2) hold for this energy.

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