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Crossings and writhe of flexible and ideal knots

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The data of ideal knots [Nature, **384**, 142 (1996)] are reanalyzed and the average crossing number of the ideal knots $\langle X\rangle_{ideal}$ shows a nonlinear behavior with the essential crossing number C. Supplemented with our Monte Carlo simulations using the bond fluctuation model on flexible knotted polymers, our analysis indicates that $\langle X\rangle_{ideal}$ varies nonlinearly with both C and the corresponding average crossing number of the flexible knot, which is contrary to previous claims. Our extensive simulation data on the average crossing number of flexible knots suggest that it varies linearly with the square root of C. Furthermore, our data on the average writhe number $\langle \mathrm{Wr}\rangle$ indicate that various knots are classified into holonomous groups, and $\langle \mathrm{Wr}\rangle$ has a quantized linear increment with C in all four knot groups in our study.

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I. INTRODUCTION

Knots play crucial and significant roles not only in mathematics [1,3], but also in physics and biomolecules [4–13]. Mathematicians have studied knots since the 19th century, but physicists only for the last few decades. In mathematics, the classification of knots is one of the most important problems [1,2]. In biology, DNA could appear as knotted DNA during replication processes with the help of enzymes [11,12]. Also, knotted DNA undergoing gel electrophoresis could help biologists to identify what type of knot the DNA is [14]. Also, knotted structures in proteins may provide some clues to their folding processes [15]. Therefore, understanding the topological effects of knotted polymers is of both fundamental and practical importance. The geometric and physical properties of flexible knotted ring polymers was studied by some authors [16–25]. The relation between topological invariants and the static and dynamic quantities of knotted polymers, i.e, radius of gyration and relaxation time, was investigated [18,22–25]. In order to study different types of knotted ring polymers, seeking suitable quantities that can identify the knot type is of practical importance. The most commonly used and intuitive one is the essential crossing number C, which is the minimal number of crossings when the knot trajectory is projected onto a plane. The notation we used for knot types is the standard Alexander-Briggs notation [2]. Figure 1 shows some knots in their standard projections, with minimal crossings. Traditionally, knots are labeled C_K, where C is the number of essential (or minimal) crossings no matter how the knot is topologically deformed without cutting it; K is just a label to distinguish topologically different knots. For the purpose of distinguishing topologically different knots, C is not an effective quantity because there are many topologically different knots having the same value of C. However, the number of crossings of a knot projected on a plane (which is $\geqslant C$) is still a physically useful quantity, since it shows how entangled the polymer is, at least in an average sense. Especially from the viewpoint of polymer physics, the average crossing number X (i.e., the average number of crossings when the knot is projected and averaged over all directions) reflects the interactions among the segments. Unlike C, X is a real number and not a topological invariant.

Another important topological quantity to characterize a knot is the writhe of a knot. In simple words, writhe is the sum of all signed crossings when we view the knot from a certain direction. There are basically two common notions of the writhe of a knot, namely, the topological writhe w and the average writhe Wr (the writhe average over all directions, called three-dimensional writhe in Ref. [26]). The topological writhe w (also known as the Tait number) is the sum of all signed crossings when the knot is projected onto a plane

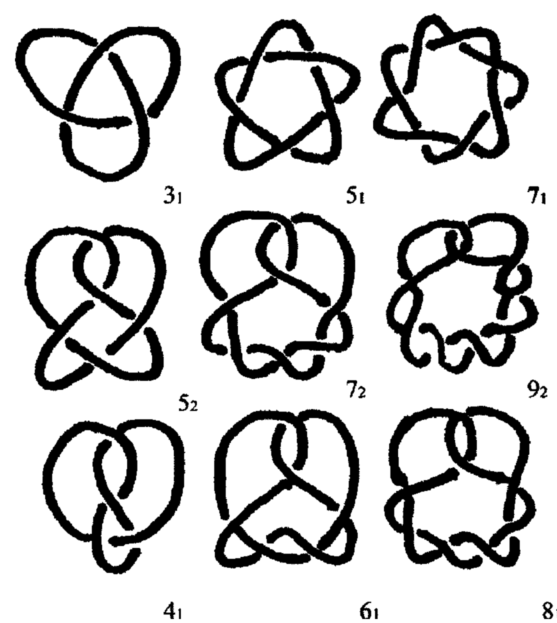

FIG. 1. Knot diagrams for various prime knots.

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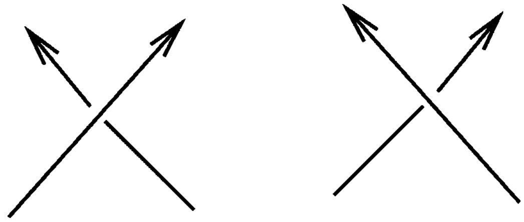

FIG. 2. Sign convention of the writhe of a crossing. Left: $+1$; right: -1

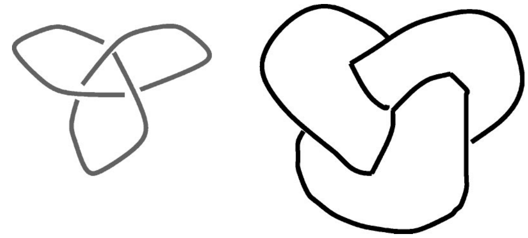

FIG. 3. Left: Standard projection knot diagram of the trefoil 3_1. Right: Maximally inflated ideal knot of 3_1.

with minimal crossings. Imagine a certain direction is assigned to the knot as one traces along the contour length; then, as the knot is projected on a plane, each crossing can have two possible configurations, as shown in Fig. 2. The sign convention of $+1$ and -1 crossings is shown, and w is just the algebraic sum of all these $+1$'s and -1's. Just like the essential crossing C, w is an integer, and is a topological invariant for a given knot type. The first column in Table I gives the values of w for various knots in this study. Both w and Wr can be used to characterize the chirality of a knot. A knot is achiral (i.e., it is topologically identical to its mirror image) if and only if $w=0$ (and also $\mathrm{Wr}=0$). However, Wr can quantify the chirality of a knot more effectively, since it is an average quantity which takes real values and can distinguish different knots better. Katritch *et al.* studied the average writhe of ideal knots [19], and observed a linear relation between Wr and the minimun crossing number C for some categories of knots. Similar results of a linear variation of Wr with C for torus flexible knots on a cubic lattice up to nine essential crossings were also observed in Ref. [27].

Instead of flexible knots, the notion of ideal knots (tight knots) and their geometrical properties has attracted much interest in recent years [18–20,28,29]. The so-called ideal knot is the tightest knot for a given rope. That is, for a given diameter of a rope, the ideal configuration of the knot is defined to be the one with the shortest contour length. Instead of C, a new topological invariance p has been used, which is defined as the length to diameter ratio of the knot at its maximally inflated state [18], to identify knots. The value of p measures the complexity of a knot, and it could distinguish knots somewhat better than C, but on average p varies linearly with C. Figure 3 is a schematic representation of an ideal 3_1 knot. Katritch *et al.* studied the average crossing number and writhe of ideal knots up to $C=11$ minimum crossings [19], and they also studied the torus ideal knots up to $C=63$ [30]. Finally, they observed a linear correspondence between the average crossing number of ideal knots and thermally equilibrated flexible DNA knots. Thus it was proposed that the average shape of knotted flexible polymeric chains in thermal equilibrium is closely related to the ideal knots of a corresponding knot type in the sense that the average crossing numbers of the ideal and flexible knots are linearly related. In order to investigate the relation between the properties of ideal and flexible knots, a more detailed and complete study is needed. For instance, the average crossing number of ideal knots has been claimed to show a linear correlation with p [19]. However, after further studies on more complicated ideal knots of a torus, it was found that the relation between the average crossing number and p no longer follows a linear relation [30]. In this paper we shall reanalyze the data on ideal knots in Refs. [19,28] in terms of the essential crossings C, and clarify these issues by performing simulations on flexible knotted polymers using a different model.

II. MODEL AND SIMULATION DETAILS

We study the knotted polymers up to a minimum crossing of 20: $3_1, 4_1, 5_1, 5_2, \dots, 20_1$. The knot diagrams of some of

TABLE I. Table showing the different knot groups in this paper with their Alexander polynomials $\Delta(s)$ and Conway notations [2]. C is the number of essential crossings in the knot.

Knot Group	w	w_x	w_y	$\langle \mathrm{Wr} \rangle$	$\Delta(s)$	Conway notation
$(2,C)$ torus knots						
$(3_1, 5_1, 7_1, \dots)$	C	$C-1$	1	$\frac{10}{7}C-\frac{6}{7}$	$(1+s^C)/(1+s)$	C
Even twist knots						
$(4_1, 6_1, 8_1, \dots)$	$C-4$	0	$C-4$	$\frac{4}{7}C-\frac{16}{7}$	$\frac{C}{2}-1-(C-1)s+\left(\frac{C}{2}-1\right)s^2$	$(C-2)(2)$
Odd twist knots						
$(5_2, 7_2, 9_2, \dots)$	C	2	$C-2$	$\frac{4}{7}C+\frac{12}{7}$	$\frac{C-1}{2}-(C-2)s+\frac{C-1}{2}s^2$	$(C-2)(2)$
$(6_2, 8_2, 10_2, \dots)$	$C-4$	$C-4$	0	$\frac{10}{7}C-\frac{40}{7}$	$-1+3s\left(\frac{1+s^{C-3}}{1+s}\right)-s^{C-2}$	$(C-3)(1)(2)$

the prime knots we study are shown in Fig. 1. We have chosen all the knots with non-negative topological writhe values. The values of the writhe of a knot and its mirror image differ by a factor of -1. The simulation model we used is the bond fluctuation model [31]. The bond fluctuation model is a coarse-grained model of polymers; monomers are put on sites of a cubic lattice. All the detail excluded volume interactions are modeled as a nonoverlapping of monomers. N monomers are sequentially connected by bond vectors to form a ring polymer. Bond vectors are only allowed in the permutation set of $\{(\pm 2,0,0),(\pm 2,\pm 1,0),(\pm 2,\pm 1,\pm 1),(\pm 2,\pm 2,\pm 1),(\pm 3,0,0),(\pm 3,\pm 1,0)\}$; therefore, bond crossing are forbidden, and the topology of the polymer knot could be preserved. For each Monte Carlo move, a monomer attempts to move randomly to one of its nearest neighbor lattice sites. The trial move is accepted if the excluded volume is obeyed and the new bond vectors still belong to the allowed set. In our simulation of flexible polymer knots, the initial knot configurations are well equilibrated for several million Monte Carlo steps per monomer. The measurements of the average crossing and writhe are then taken over about ten times of the equilibration time. Thermal average is denoted by $\langle \cdots \rangle$. Various knot groups, listed in Table I for chain lengths up to $N=240$, are studied. The writhe number Wr is calculated as [32]

$$\mathrm{Wr}=\frac{1}{4\pi}\oint\oint\frac{(\vec{r}-\vec{r}\,')\cdot d\vec{r}\times d\vec{r}\,'}{|\vec{r}-\vec{r}\,'|^3}, \tag{1}$$

where the integrals are integrated along the contour of the knotted ring polymer. The average crossing number is calculated in a similar way [19], by the integral

$$X=\frac{1}{4\pi}\oint\oint\left|\frac{(\vec{r}-\vec{r}\,')\cdot d\vec{r}\times d\vec{r}\,'}{|\vec{r}-\vec{r}\,'|^3}\right|. \tag{2}$$

The mean contour length of the flexible knot is also measured, and we ensure that the knot is far from being tight. In most cases, the mean contour length of the flexible knot is almost the same ($<1\%$) as the circular unknot 0_1 with the same N.

III. AVERAGE CROSSING NUMBER

Here the average crossing number measured for an ideal knot is denoted as $\langle X\rangle_{ideal}$, while the average crossing number of a flexible knot is without the subscript. Figure 4(a) is a replot of the data in Ref. [19] on the average crossing number versus C for ideal and flexible knots of 5400bp DNA. $\langle X\rangle$ for the flexible DNA appears to curve away from a linear relation with C. To confirm this nonlinear behavior, we independently perform simulations for flexible knots using the bond fluctuation model for knotted polymers of $N=180$ and 240. The results are shown in Fig. 4(b). It is quite obvious that a strictly linear relation between the $\langle X\rangle$ and $\langle X\rangle_{ideal}$ does not hold. Furthermore, by fitting the data in Ref. [30] up to $C=63$ for ideal knots, as shown in Fig. 5, we empirically find that the power law $\langle X\rangle_{ideal}\propto C^{1.2}$ can describe these data on ideal knots very well. The data for the

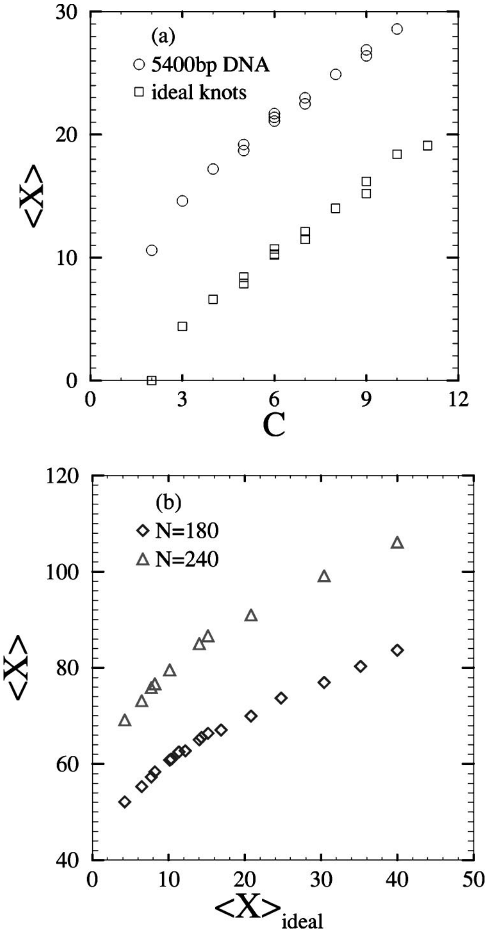

FIG. 4. (a) $\langle X\rangle$ vs C for ideal knots and 5400bp DNA flexible knots. (b) Mean crossing number for the flexible knots $\langle X\rangle$ vs the mean crossing number of the corresponding knot in its ideal configuration $\langle X\rangle_{ideal}$. Values of $\langle X\rangle$ are from our simulations of the bond fluctuation model. Values of $\langle X\rangle_{ideal}$ and DNA data are taken from Refs. [19,30].

average crossing number of various flexible knotted polymers are analyzed, together with the data of 5400bp DNA, and are depicted in Fig. 6. It appears that the average crossing number of flexible knotted polymers is consistent with a linear variation of the square root of the minimum crossing number $\langle X\rangle\sim\sqrt{C}$. This result is quite different from those for ideal knots which behave as $\langle X\rangle_{ideal}\propto C^{1.2}$. In Ref. [19], knots were studied only up to a crossing to 11, and the average crossing numbers of ideal and flexible knots seemed to be linear. However, the study of torus knots up to 63 crossings in Ref. [30] provided a clue to this nonlinear relation. As in our study, the knots are more complicated, and are from various families up to 20 crossings; the nonlinear behavior is shown explicitly. Figure 4(b) displays the average crossing numbers of ideal knots and flexible knots; in contrast to the results in Refs. [19,28], the nonlinear tendency could be seen explicitly.

We further examine the excess average crossing number of a flexible knot $\langle\Delta X\rangle$, defined as the difference of average crossing numbers between a given knot type and the trivial knot 0_1 with the same N. In Fig. 7, $\langle\Delta X\rangle$ is plotted against

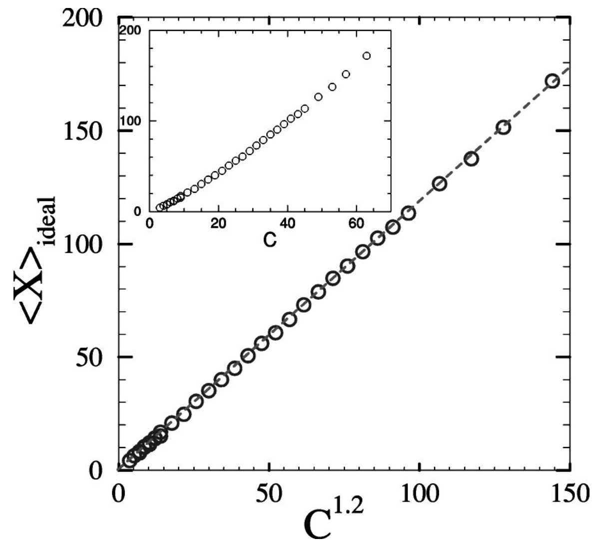

FIG. 5. The mean crossing number of ideal knots plotted against $C^{1.2}$. Inset: $\langle X\rangle_{ideal}$ vs C. Data are taken from Ref. [30].

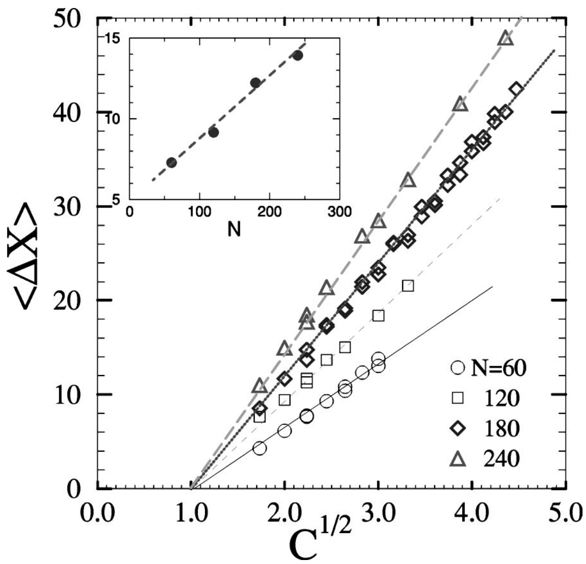

FIG. 7. Mean excess crossings plotted against $\sqrt{C}$ for flexible knots of various lengths. Inset: the slopes of the fitted straight lines (α_N) vs N. Straight lines are best fits to the data.

$\sqrt{C}$ for different flexible knots with various lengths. The variation of $\langle\Delta X\rangle$ follows a linear behavior with $\sqrt{C}$ for a given N; moreover, the lines for different values of N all intersect at the same point. This suggests a relation of the form

$$\langle\Delta X\rangle=\alpha_N(\sqrt{C}-1), \tag{3}$$

where α_N depends on N. Furthermore, the slope α_N increases with N as expected, and appears to have a roughly linear dependence on N, as shown in the inset of Fig. 7.

IV. LINEAR INCREMENT OF THE MEAN WRITHE

In this section, we focus on the results of mean writhe number of ideal and flexible knots. Comparing the average writhe number of ideal knots with flexible knots, they are numerically very close, as shown in Fig. 8. The reason for the almost identical values of $\langle\mathrm{Wr}\rangle$ for ideal and flexible knots can be understood as the following: each snapshot configuration of a flexible knot of a given type, is topologically equivalent to an ideal knot of the same knot type; hence the flexible knot can be obtained by lengthening the ideal knot to the appropriate contour length, and then followed by several Reidemeister moves [2–4]. For the second and third Reidemeister moves, the net writhe number gain is zero. For the first Reidemeister move, the writhe number increases or decreases by 1 depending on the right or left-handed crossing so produced. But the right- and left-handed crossings have an equal opportunity to occur, since flexible knot configurations result from a random thermal motion, so the mean writhe number $\langle\mathrm{Wr}\rangle$ is unchanged after averaging. Therefore, ideal knots could represent flexible real knots for the average writhe number, but not for the average crossing number as we discussed previously. It is worth noting that the value of

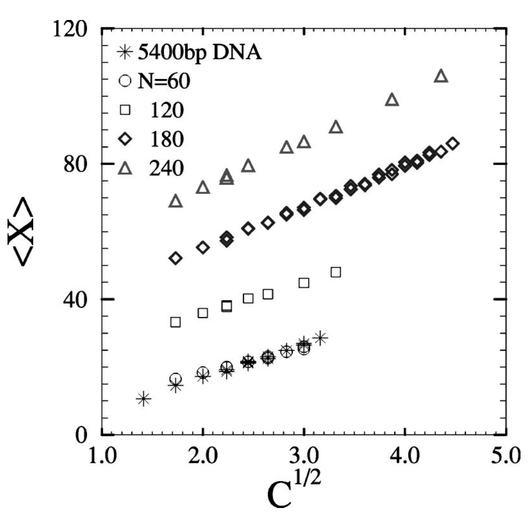

FIG. 6. Mean crossing number of flexible knots vs $\sqrt{C}$ for knots of various lengths. Data for the DNA are from Refs. [19,30].

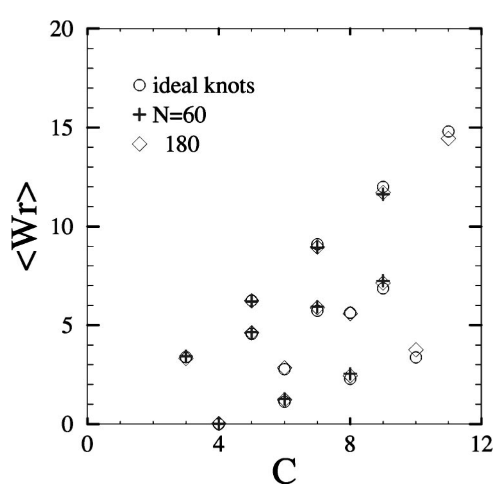

FIG. 8. Mean Wr vs C for ideal knots and flexible knots. Data for the ideal knots are from Refs. [19,30].

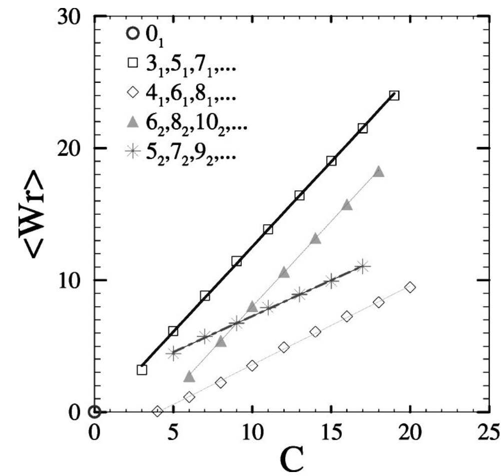

FIG. 9. Mean writhe $\langle \mathrm{Wr} \rangle$ vs C for various flexible knots. All data are with $N = 180$. Uncertainties are much less than the sizes of the symbols.

$\langle \mathrm{Wr} \rangle$ is independent of the knot contour length (see Fig. 8), and thus represents a scale independent topological feature of the knot type.

Another interesting result is the dependence of $\langle \mathrm{Wr} \rangle$ on C, which is shown in Fig. 9. The data indicate a natural categorization of the knots in this study into four types. Knots $3_1, 5_1, 7_1, \ldots$ belong to the family of torus knots. Knots $4_1, 6_1, 8_1, \ldots$ are twist knots with even number of crossings. Knots $5_2, 7_2, 9_2, \ldots$ are twist knots with an odd crossing number. These groups are known as holonomous families to knot theorists. That knots are classified into groups by the mean writhe number is not too surprising, because each of these knot groups has topological properties in common with the others. This is clearly reflected by the parametrization of their Alexander polynomials and the Conway notations within each group. Table I displays these knot invariants for the four knot groups in this study. The linear relationship between the average writhe number and the minimum crossing number within each knot group is even more astonishing.

Such a linear increase of $\langle \mathrm{Wr} \rangle$ within a holonomous knot group was also observed recently in simulation studies of torus knots on a cubic lattice [27] and ideal knots [19] up to $C = 11$, and for three knot groups (torus, even, and odd twist knots). Our results show explicitly that such a linear behavior is universal in the sense that different polymer models (such as ideal knots, cubic lattice knots and bond-fluctuation models) have the same behavior. Furthermore our data (Fig. 9) indicate that such a result holds at least up to $C = 20$, and is also valid for the $6_2, 8_2, \ldots$ group. Although there is yet no theoretical understanding of the origin of such a linear increment of $\langle \mathrm{Wr} \rangle$, Cerf and Stasiak attempted to summarize such a linear behavior of the data of $\langle \mathrm{Wr} \rangle$ of ideal knots in terms of topological invariants by an empirical formula [26]

$$\langle \mathrm{Wr} \rangle = \tfrac{10}{7} w_x + \tfrac{4}{7} w_y = w + \tfrac{3}{7}(w_x - w_y), \qquad (4)$$

where w is the topological writhe mentioned before. w_x and $w_y = w - w_x$ are the nullification writhe and remaining writhe, respectively. Both w_x and w_y are topological invariants, and take integer values. Table I displays the values of these invariant writhes in terms of C for the knot groups in this study. When w and w_x are translated in terms of C, the empirical formula [Eq. (4)] implies that $\langle \mathrm{Wr} \rangle$ is a linear function of C, and is tabulated in Table I for each knot group. From the empirical formulas in Table I (fifth column), the slopes of the even and twist knots are the same $(10C/7)$, while the slopes of the other two groups take the same values of $4C/7$. Our data indicate that the empirical formula holds rather well, although there are still some noticeable small deviations. For example, for 7_2 and 8_2 knots, Eq. (4) predicts them to be the same with $\langle \mathrm{Wr} \rangle = 40/7 \simeq 5.714$, but our results indicate that a $\langle \mathrm{Wr} \rangle$ of 7_2 is larger than one of 8_2; the difference, though small, is larger than the estimated uncertainty.

$\langle \mathrm{Wr} \rangle$ measures the average chirality of a knot, or the degree of mirror asymmetry, as the knot is viewed from all directions. In a certain sense the value of $\langle \mathrm{Wr} \rangle$ is governed by the detailed topological interactions among the segments in the knot. The similarity of the detail topology within a group will hence classify the values of $\langle \mathrm{Wr} \rangle$ into different knot groups, as shown in Fig. 9. Presumably the principal portion of these topological interactions gives rise to the nice linear behavior of $\langle \mathrm{Wr} \rangle$ within a group as given by the fifth column in Table I, or Eq. (4). The small deviations from Eq. (4) are possibly due to the fine structures of the topological interactions, which results in observable corrections from the principal topological interactions. In fact, in a recent study of nonequilibrium relaxation of a cut knot [33], it is observed that such a natural classification into the same knot groups also occurs in a nonequilibrium relaxation time which also has a linear variation with C within a group.

V. SUMMARY

By extensive simulations we have studied flexible knots up to a crossing of 20. Our results show that the relation between average crossing numbers of ideal and flexible knots is nonlinear, which disagree with the claim that ideal knots could represent the physical properties of flexible knots. Our data also suggest that the excess average crossing number for flexible knots behaves as $\langle \Delta X \rangle = \alpha_N(\sqrt{C} - 1)$. The coefficient α_N increases roughly linearly with N. The average writhe number $\langle \mathrm{Wr} \rangle$ of a flexible knots is found to be numerically the same to its corresponding ideal knot, and is length independent. Thus the ideal configuration of a knot can truly represent some properties of a flexible knot, such as the mean writhe. However, for some other geometrical or physical properties, such as the mean crossing numbers, the ideal configuration may not be that useful, as they are nonlinearly correlated for the ideal and flexible knots. $\langle \mathrm{Wr} \rangle$ naturally classifies knots into holonomous knot groups with similar detail topologies. More remarkable is the quantized linear increment of $\langle \mathrm{Wr} \rangle$ with C within each holonomous group. Such a linear law is quite well obeyed and presumably arises from the average intrinsic topological interactions from the entanglement within the knot.

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