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Is quantum computing promising for soft matter problems?

Polymer physics by quantum computing
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In the last few years, I had an opportunity to ask every new incoming graduate student in our Physics Department at New York University – which branch of physics attracts them most? Surprisingly, year after year, six or eight of every ten aspiring physicists replied something along the lines of quantum information, quantum computing, etc. Of course, seasoned physicists look in this direction, too. Today, most of the efforts in the field seem to be revolving around the use of programmable quantum simulators as potentially versatile platforms for studying many-body phases and dynamics in strongly interacting quantum systems.

In the recommended paper, C.Micheletti and his co-authors ask a very different question: if a quantum sorter was available today, what kind of long standing tough classical polymer physics and soft matter problems could it solve? Authors illustrate their idea using a specific example – chosen, in my opinion, with a great taste. The beauty of the example is that it does not involve any parameters, arbitrary or adjustable ones – none.

To explain the model and why it is so interesting, let us start with a long flexible polymer chain whose ends are glued together, such that the chain forms a loop. As one can readily surmise from the experience with (wired) headphones, or charging cables, or fishing lines, or any other object of this kind, when you randomly glue together two ends of a long polymer chain, the resulting loop, with overwhelming probability, is heavily knotted. Indeed, it is a proven mathematical theorem [1] that the probability to have no knots in a looped polymer of length N units, in the large N limit, goes as $\sim \exp\left[-N/N_0\right]$, where N_0 is a unitless parameter that depends on the type of the polymer. Alas, it does not mean we can forget about long unknotted loops, because there are processes in nature, and especially in the living cell, that make such loops with no knots (or some similar objects). But understanding of such objects is challenging. Indeed, the exponentially small probability of unknots in a random loop means that forcing loop to have no knots places it in an exponentially small "corner" of the configuration space. In other words, examination of equilibrium statistical mechanics of the unknotted loops one has to perform the summation over an exponentially improbable set of

Figure 1: Rubber bands from a local supermarket illustrate the linked configurations of topologically unconcatenated rings.

conformations delineated by their topology. There are no regular mathematical methods to do it.

But now imagine that instead of one such unknotted loop, we have many. They are not concatenated to one another, adding one more level of topological complexity. This model of many unknotted and unconcatenated loops densely packed together is known as a melt of unconcatenated and unknotted polymer rings. As a model, it is quite well known one. For simplicity, it can be realized on a simple cubic lattice, with the only interaction between non-connected monomeric units is the self- and mutual-avoiding condition (excluded volume). Rings are made of flexible chains, meaning that continuing straight and turning 90 degrees (the only options on the cubic lattice with avoidance) have the same energy – which is why the model is truly parameter-free.

This model, of course, was examined before in numerous theoretical and simulation papers. Although current consensus seems to be stalled at the point of everybody assuming that every ring in such melt is characterized by the compact size scaling $\sim N^{1/3}$, this conclusion is based on an admittedly weak computational evidence [2] and some theoretical arguments which are difficult to make rigorous [3, 4]. At the same time, there is no doubt that in a large system, some of the rings will adopt some less trivial topological configurations (while still remaining strictly unconcatenated!). I illustrate some of the possibilities with rubber bands that are used in a local supermarket to pack produce – see Fig. 1. Although the probabilities of such configurations in equilibrium are almost certainly exponentially small (at $N \gg 1$), but, very importantly, each of them gives an exponentially large contribution to some of the correlation functions and related quantities such as zero shear viscosity. Therefore, these conformations in the end might prove very important. Incidentally, they are indeed observed in a strongly non-linear regime of an extensional flow [5]. Not going to any details, I mention also an appealing but controversial idea of a "topological glass" [6, 7, 8, 9, 10].

And here comes C.Micheletti with his co-authors, as they devise a beautiful algorithm that should be possible to implement – once a quantum sorter could be purchased in a convenience store around the corner. Their algorithm does seem to be able to solve the problem once and for all. Of course, it is a little disappointing that in the end of the exercise

we still don't know the answer to the physics question – but we have a plan on how to find out.

Of course, the model by C.Micheletti et al can be "improved" by including some parameters, such as, e.g., bending rigidity of the chains; in my opinion, this would be a counterproductive approach at the present stage, when we don't actually solve the problems, but only devise algorithms to do it in the future.

Thinking along the lines of the original parameter-free model, I am tempted to suggest another potentially interesting group of polymer physics model, where the key is the search through exponentially large space. In this case, I am thinking of heteropolymers (or copolymers), say, of two types of monomers, A and B. There are, of course, 2^N possible sequences and it is very likely that some of these sequences offer and exponentially large thermodynamic advantage over the others. Allowing myself a wild speculation, I can suggest that perhaps "successful" biopolymers represent such exponentially improbable subset of all. Maybe, quantum sorters can help us understand something fundamental there? Perhaps some of the graduate students, declaring their interest in quantum computing, should start thinking in this direction.

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