ATIF JAVED: Hey, 3016. Welcome to my final video project for the class. My presentation will be on Modeling and Energy Analysis of Liquid Crystals using Mathematica.

So liquid crystals pervade many areas of technology in our world today, including the screen you may be watching this on. They're used in LCD displays, thermometers, surfactants, polymers, detergents, and even Kevlar. So the versatility of this phase of matter is what definitely piqued my interest and made me especially enthusiastic about this project as an opportunity also to explore this subject as a scientist would, imposing my own questions and then finding ways to answer them.

So let's move on to the subject matter. Liquid crystals are the state of matter which retains properties from the conventional crystalline solid and the isotropic liquid state. So here you see an example of the crystalline solid.

LC molecules are anisotropic, meaning that they exhibit properties with different effects when oriented in varied directions. And that orientation implies a certain free energy. And that allows for a structure with interesting properties, such as let's say birefringence.

So here we see the entire disorder of an isotropic liquid. And as we move right, we're removing degrees of freedom to eventually form nematic LCs that have orientational order, and eventually smectic LCs, which have both orientational and translational layering order, which, by the way, is growing as a tool in research, especially in nanotechnology and high-performance materials, which I thought was pretty cool.

Everything ultimately references back to structure. And here we can see the increasing degrees of freedom and the characteristic decreasing order parameter value as we transition to a liquid. So the transitional degree of freedom but restricted rotational freedom is what will guide our assumptions in developing a strong model.

All three subdivisions of the liquid crystal phase can exhibit phase transitions, because of temperature fluctuations. So this will motivate my analysis of the energy and entropy, which are directly based on the order of the system, and whose order is different based on the temperature. So I will be using calamitic, or rod-shaped, liquid crystals, and finish my analysis with a statistical modeling of the energy and entropy over 100,000 trials, and examine the graphical representation.

So since the molecules are calamitic, I can think of them basically as straight rods. Thus, the orientation is only based on the beginning and the end of the rod. So because we'll be looking at trends, we can simplify the problem by first approaching it in two dimensions.

And after a ton of trial and error, I was able to put together a graphic of these rods to shape the order of our liquid crystal system, and demonstrate the type of phase that we're in. And it's defined by the average theta angle from the order director. And this is the random generator for our LC system, where we can change the theta value for our director. And from this, we can work on extrapolating energies in them.

So here, we show three primary energy scenarios for non-polar crystals. And what can be considered their relative energy is given by this equation at the top. So by setting these conditions, when molecules are parallel that gives a relative interaction energy of negative 1; and when perpendicular, a net energy of 0l and when angled 45 degrees to the director, yields an energy of about negative 0.5.

So we can keep the negative sign as we take the dot product of the two directions to represent the fact that a lower free energy corresponds to greater stability in either translation or orientation. But we'll keep things positive for our graphics in the future.

So we can consider the molecules to be on average equidistant from one another. And so we can grid our liquid crystals in 2D space, like so. Then we can visualize how the nearest neighbors, particularly the ones in directly adjacent cells, affect the energy of the system. The energy effects of molecules farther than these adjacent ones can be considered negligible in comparison to these closer ones.

So we further our model by taking the summation of energies in the necessary locations, ultimately assigning a total energy to each crystal that encompasses the energy of that crystal resulting from orientation. Or other energy contributions could exist, let's say, such as magnetic. But we'll focus on the energy of order and the results from bonding and lowering of entropy.

Now subsequently, we can create a collection of data angles produced from 100,000 trials of our random liquid crystal generator, and obtain their energies from the relationships described earlier. So from this, we can develop a histogram, as shown here in the top right-- in the top left. And we clearly see it is relatively uniform Gaussian distribution, as expected.

So moving forward, we want to look to the third law of thermodynamics to relate what we are seeing to entropy using a fundamental law. And so we'll graph our energy against entropy using the natural level omega multiplied by the Boltzmann constant. Omega is the number of microstates, i.e., the number of configurations, basically, that are still macroscopically a liquid crystal.

So by taking the log of our first graph, we can obtain the second one plotting energy versus entropy. And we see the curve flattens by taking the natural log of the states. And so after normalizing, we get the same graph, except slightly wider and flatter. And we can see this contrast in the lowest picture.

But now for the most interesting part of the problem, we know from the Gibbs free energy equation and the first law of thermodynamics that for an isolated system such as this, that dU equals TdS, where dU is the internal energy. And so rewriting this, we see the relationship between temperature and changing energy and entropy. And since we have developed this information from our previous graph, all we have to do is rotate the axes of S against E, making the slope of the curve equal to our temperature for whatever generated liquid crystal.

Although I was unable to create the manipulate command that would demonstrate the slope of dE versus dS as the temperature was decreased, we would expect a narrower distribution of beta angles, in other words an increase of the order of the system by being more aligned with the director, to compress the histogram and result in a lower slope for T.

And this is pretty cool. In my mind, it's a pretty cool thermodynamic proof, that the narrower distribution of rods equates to a lower temperature, and conversely, a wider distribution of rods around energies represents greater randomness, and thus higher temperature. And so with confidence, we can say that the order and temperature are mutually dependent.

And so I think the beauty of this problem really stems from the simplicity derived from taking appropriate steps and realizing where the need for comparison and trend study supersedes an unnecessarily complex setup. I'm certain that that kind of technique I'll be applying this in the future in DMSC courses. And hopefully, I can continue that in my track, in studying nanomaterials as well.

So to me, that's pretty awesome. And my thanks go out to all of you, 3016 Fall 2012, for making the class like quite an experience, granted in retrospect. But nonetheless, a really cool endeavor. And my greatest appreciations go out to Ray, Esther, and of course Professor Carter for their tireless efforts. So thank you, guys.