Building a Better Ruler

March 21, 2016

Sometimes science is less about finding the right answer and more about pinning down, as Andreas Ekström said, “how wrong do you expect this to be?”

In experimental physics, scientists present their findings with error bars: the plus-or-minus value that accounts for possible errors in the central value. Ekström, who just completed a postdoctoral appointment with UT Physics, is among the researchers who adapted this approach to theoretical physics and shared their results in the paper “**Uncertainty Analysis and Order-by-Order Optimization of Chiral Nuclear Interactions (http://dx.doi.org/10.1103/PhysRevX.6.011019)**,” published February 24 in *Physical Review X*.

The Right Ruler

Ekström explained that reliable theoretical error bars are critical to determine the significance of any comparison with data. They can help identify new relevant experiments or reveal the existence of new physics.

“You need to find out how precise and accurate your model actually is,” he said.

The purpose of uncertainty quantification is to determine these quantities. Ekström explained this concept using the simple example of a ruler.

“Let’s say you want to determine the length of this desk using a ruler,” he said, stretching out his hands along the edge of the desk in front of him. “You can measure many times with this ruler and you’re going to get a slightly different number each time.”

The more times you measure, the more different values you get. This is what we call the statistical uncertainty. It comes from repetition and quantifies the precision of your result. This spread in values generally decreases with the number count.

“Now,” he continued, “it could also be that your ruler is wrong. In theoretical physics, that means that your model is wrong. So each time you compute something, you’re going to make the same mistake. That’s the systematic uncertainty and it quantifies the accuracy of your result. To estimate these two sources of errors (statistical and systematic): that’s what uncertainty quantification is.”

Owing to a strong mathematical framework, the statistical uncertainty is the easiest to quantify, while the systematic uncertainty is tougher to nail down.

“You really need to understand what you’re doing,” Ekström said. “You can compare several different theories, but there’s no simple recipe for that. You can also do several different types of measurements or calculations, which basically corresponds to comparing your results with someone else that is measuring with another ruler. We are currently developing improved methods to carefully determine the statistical and systematic errors in ab initio nuclear theory. In the long run, this will help us to include the correct physics in the models of the atomic nucleus. Or in other words, have the right ruler.”

Missing Physics

The *Phys. Rev. X* paper gives researchers in nuclear physics a better tool to assess the accuracy of the theoretical models of the atomic nucleus. Specifically, the authors present the first common statistical analysis of two key theoretical frameworks: ab initio many-body methods and chiral effective field theory.

"In fundamental nuclear physics right now, those are the dominating paradigms," Ekström said. "The interaction is described using chiral effective field theory, and scientists use that framework in ab initio solutions of the Schrödinger equation. In ab initio nuclear theory, it has not been fully investigated what the systematic and statistical uncertainties of the predictions are."

The paper shows that the systematic uncertainties in ab initio nuclear theory dominate over the experimental uncertainties.

"That brings us back to the main thing," Ekström said; "the error is most likely missing physics or poorly calibrated models or a mix of both. The published paper provides us with a tool to quantify the unknown."

Uncertainty quantification is finding its way into theory work in other scientific disciplines as well, such as neurodynamics or high-energy physics. As Ekström pointed out, "only if you have a prediction that has rather small uncertainties can you really claim to have some predictive power."

The Big Picture

Ekström has been affiliated with UT for a year and half, but has been involved with uncertainty quantification for several years. The paper itself is a tribute of sorts to the nature of physics: how it builds on years of earlier studies and develops rich collaborative relationships that cross borders. Chalmers University of Technology in Sweden was heavily invested in the work, which was led by Ekström's Ph.D. student there, Boris Carlsson, and included contributions from Christian Forssén (who spent last year at UT) and four undergraduate students. Other UT connections in the author list are former postdocs Kyle Wendt and Gustav Jansen (who is now on staff at Oak Ridge National Laboratory).

"UT has very, very strong involvement in this," Ekström said. "The predictions for heavy nuclei that we have made were carried out here. That could not have been done without involvement from Gustav Jansen."

UT Physics Professor Thomas Papenbrock and Adjunct Assistant Professor Gaute Hagen were also involved in scientific discussions on the paper, and will visit Chalmers in June, where Ekström is joining the faculty as an assistant professor this spring. He is particularly proud of the work the four bachelor's students (who are co-authors of the paper) did to develop computational tools that other users can adopt for their own studies. This community mindset is part of why the authors chose to submit their work to *Physical Review X*, which has an open-access publishing model. The American Physical Society journal publishes exclusively online, and due to its high selectivity, only publishes about 200 papers per year covering all areas of physics for broad dissemination and high visibility. Ekström and his colleagues considered it to be the best vehicle to share the promise of uncertainty quantification for nuclear theory.

"This is what this all boils down to: to learn what information is hidden in different measurements and how to best use that to constrain your theories and get hints of, perhaps, missing physics" he said. "That's the big picture."

- **Chalmers Release (in Swedish) (http://www.chalmers.se/sv/institutioner/fysik/nyheter/Sidor/Chalmersforskare-avslojar-osakerheten-i-teoretiska-modeller.aspx)**
- *Physical Review X*: **Uncertainty Analysis and Order-by-Order Optimization of Chiral Nuclear Interactions (http://dx.doi.org/10.1103/PhysRevX.6.011019)**