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NICS

Atomic Physics on Kraken

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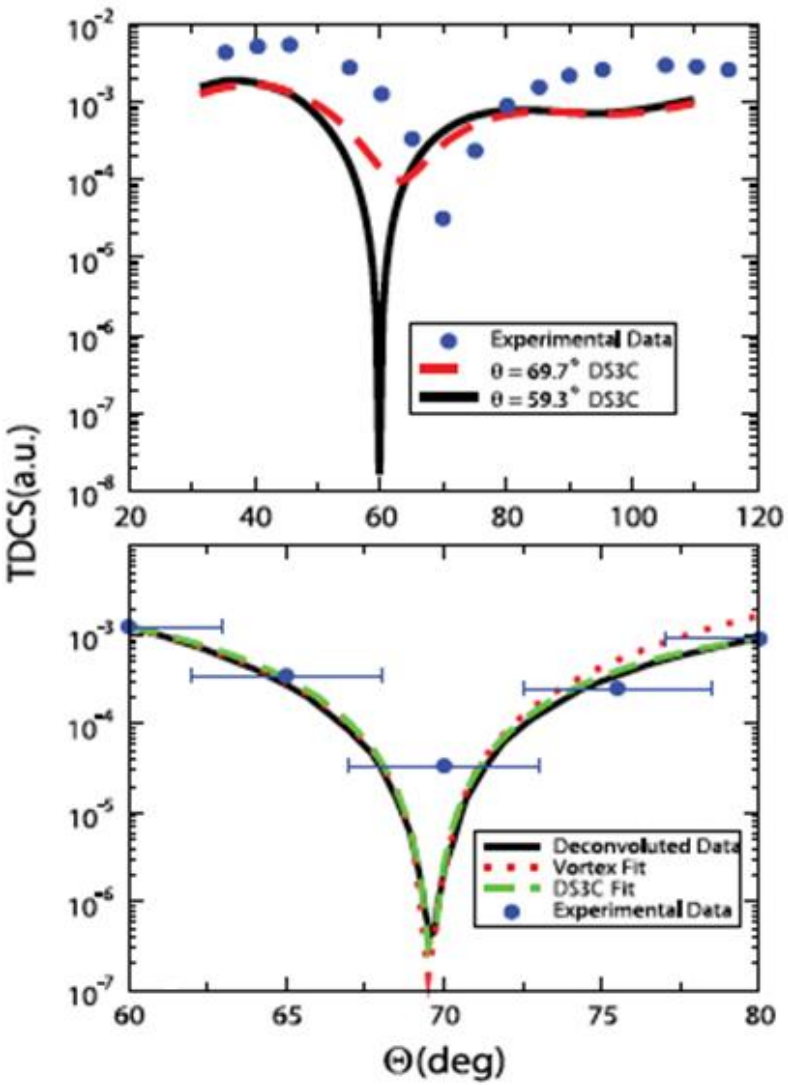
Atomic Physics on Kraken

- Great progress has been made in creating a truly quantum mechanical 4-dimensional code for atomic collisions with two active electrons. This program is currently in the testing phase and will be used to collaborate with a reaction microscope group in Germany so that they may look for the vortices that we have been predicting should appear in their data
  - The code has been ported over the simple version of the Fermi shuttle code that I have been using. A presentation of this will be made at a conference in one month with a paper soon to follow
- All of our work on Kraken has been done with only 300–500 cores in multiple 24 hour runs. I will discuss why we are using so few cores below in the "Next Steps" section
- We are currently gearing up for full-scale 4D collision calculations as well as more elaborate Fermi shuttle calculations
- Eventually, if we can utilize memory more efficiently, we would like to perform the first true 6-dimensional atomic collision calculation. This would allow us to explore processes for which all of the current theories fail at making correct predictions

Atomic Physics on Kraken (continued)

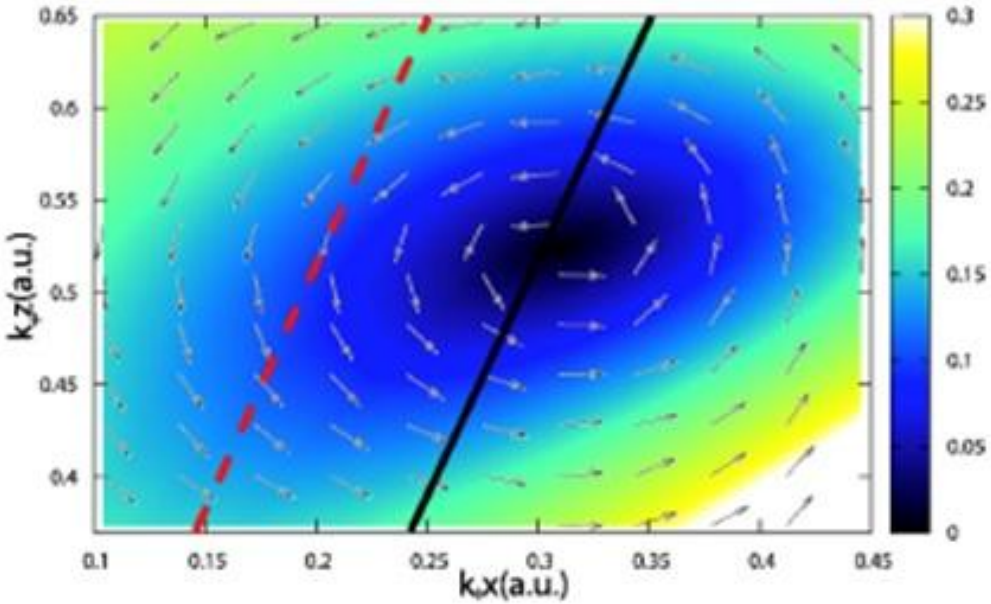
- Our main impediment to performing very large-scale calculations is lack of memory. Our code relies on highly optimized parallel FFTs. Kraken has worked spectacularly for performing these in terms of processing power. The problem that we have is that all of the available FFT routines distribute the matrix being transformed along only one dimension of the matrix. As a result, each node still has to carry a very large matrix in its memory. I have seen discussions of other distribution methods which would work much better on a large computer such as Kraken, but there are no details about how these are actually done. If we can solve the memory problem, we can do much larger calculations
- Project productivity
- Recent presentations? Recent publications? http://prl.aps.org/abstract/PRL/v104/i3/e033201

Helium

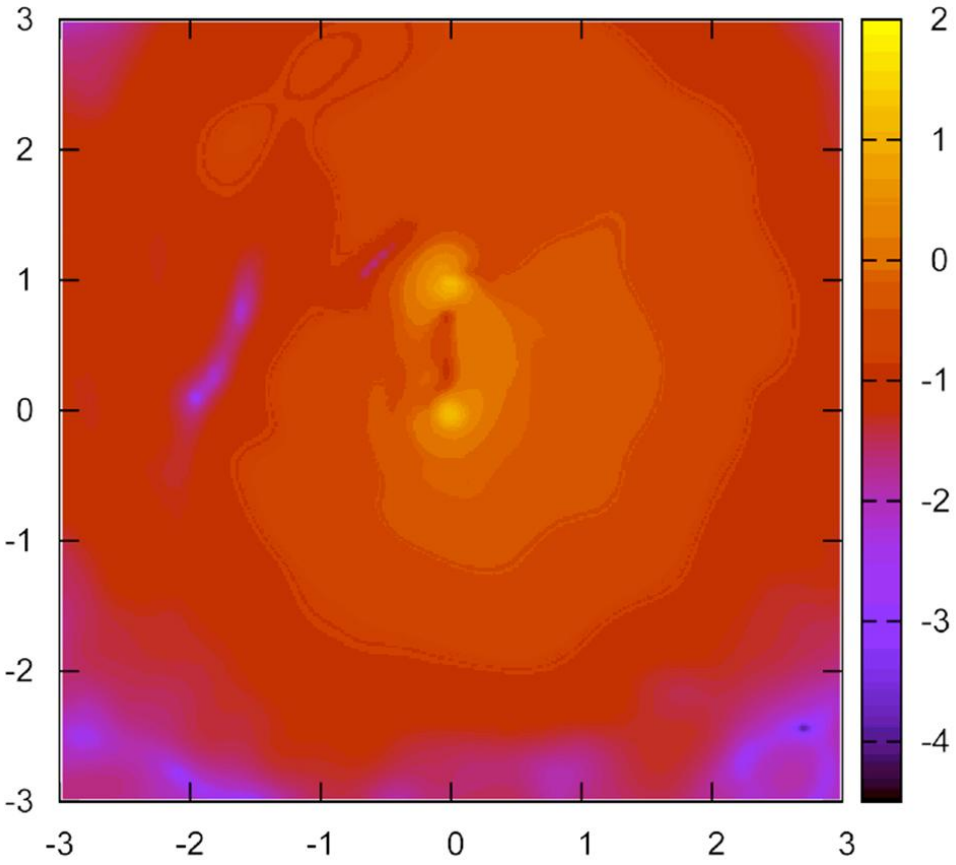


The experimental results for He(*e, 2e*)He$^+$ with $E_a = E_b = 20$ eV and $\theta_+ = 67.5°$ from Ref. [13] (blue dots) compared with the TDCS calculated using the DS3C wave function (red dashed line). Also shown is a theory curve for $\theta_+ = 59.3°$ which goes through the DS3C vortex

Comparison of the deconvoluted TDCS of Ref. [13] with a fit to the vortex of Eq. (2). The horizontal lines indicate the width of the convolution function of Ref. [13]. Also shown is a fit obtained by varying parameters in the DS3C amplitude



Contour plot of $|A(k_a, k_b)|$ on a logarithmic scale. Vectors are drawn in the direction of the current υ showing that the minimum in the previous figure is near a vortex. The diagonal lines trace the vector k_+ as the angle Θ is varied to produce the DS3C curves in the previous figure



Preliminary work being done on the two electron problem. It is done in 4 dimensions and shows several vortices

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