Article title: Time-dependent coupled-channel calculations of positronium-formation cross sections in positron-hydrogen collisions  
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Context

Often the validity and usefulness of new models in atomic physics are tested on positronium formation by positron-hydrogen collisions, as this is a simple example of an atomic rearrangement reaction with existing experimental results. Previous models are valid for low positron energies, but become non-physical at higher energies due to an over-complete basis representation. A new method of predicting atomic rearrangement exists, and involves solving time-dependent coupled-channels equations exists. This approach avoids the over-completeness problem, but requires testing to demonstrate its validity.

Purpose

The authors are trying to develop a useful implementation of the TDCC method, and determine the domain in which the TDCC model accurately predicts experimental results.

Approach

The key approaches of the paper are the applications of both a TDCC solution method, and Hankel-interpolation to calculate cross sections.

The authors expanded angular momenta into coupled channels, then present a simplified 1D framework for solving the time-dependent Schrodinger equation using this coupled-channel expansion. This essentially boils down to computational mathematical techniques. These include linearising and expanding equations to some low order, and solving on sub-intervals of some chosen small timesteps. This is shown to be solvable by numerically describing the wavefunction on grid points in the chosen space (1D for this example), and solving on these grid points.

They also describe their application of Hankel-interpolation, which is a coordinate transform. The authors are using this to transform into the ”SF representation”, which I do not fully un- derstand. They did this to subsequently solve the TDCC equations in this representation.

Contribution

The TDCC method and Hankel-interpolation were applied to calculate positronium-formation cross sections at incident positron energies of 6.8 − 50 eV. These cross sections were compared to measured cross sections from earlier experiments, as well as to cross sections calculated using different models. The cross sections calculated agree with experiment for energies less than 35 eV. At higher energies, the TDCC model under-predicts experimental results. This underestimation is explained as an effect of the limited included terms in the channel expansion for the angular momentum, which causes the error to increase significantly at high energies. This can be mitigated by increasing the number of allowed terms, and so isn’t an unsolvable issue. The authors therefore assess that the TDCC approach is viable, and could be used at higher energies if more terms are included.

Relevance

My project will be essentially solving TDCC equations for nuclear dynamics. This paper gives a clear explanation of how to solve TDCC equations for an 1D problem, and so is key to learning how to solve these equations for my project. Solving TDCC equations has never been done in nuclear physics, and so while this paper may discuss the method in the atomic physics context, it also describes the technique better than other papers. As well as describing one approach to solving the TDCC equations, alternatives are referenced for each step in the method, which will be useful in finding the best approach for the needs of my project.

Quality

I found the quality of writing and presentation of results in this paper to be good. The dense mathematical approach to solving TDCC equations in particular was well presented using a simpler 1D case. I still find it difficult to interpret due to the many different indices and terms involved, but I cannot imagine a better way of presenting the method clearly. The results were clearly stated, with a key graph presenting results on the same plot as measurements and alternative models. These results can easily be understood without knowledge of TDCC methods.

The assumptions and approach appear to be valid, as the results match well with independent experimental data. I cannot comment on the mathematical approach as I still don’t understand it, but the paper provides numerous references for each step in their process, which I can investigate when needed.

The conclusion that this model is useful appears valid to me. The model matches data well for low energies, and a clear way to improve performance at higher energies exists.

Questions/Directions

* How does the method of deriving the TDCC equations change when we move from atomic to nuclear physics? (Talk to supervisor)
* Are there any more efficient ways to numerically solve the equations? (I need to follow the references of this paper, and maybe talk to someone at the MSI)
* How can I implement this approach as a computer code, specifically in C++? (Currently attempting this)