Instructions

(1) This is the part of the semester where I have covered all the material that you will be formally tested on, and I now invite you to complete the class with a project that reflects your interests in quantum mechanics.

(2) First option: exploration of a problem in quantum mechanics using the techniques learned this semester, or even techniques that were not learned this semester, together with a numerical environment such as MatLab, Mathematica, etc. A few examples to get you thinking (not necessarily to choose from!)
   - Make a toy program to solve a model electron correlation problem, such as for two electrons in H₂ at short and long bond lengths (all the matrix elements were provided in an infamous problem set!).
   - Explore the link between wavepacket dynamics and correlation functions by making a model wavepacket rattle around in a potential (either choosing a simple form for the wavepacket and/or a simple form for the potential).
   - Look at numerical explorations of the coupling of a discrete state to a continuum to see the range of possible lineshapes, or to pursue extensions beyond the basic model treated in lectures.
   - Explore non-adiabatic transitions using the Landau-Zener model (or more advanced extensions if you wish) using some model for two state potential energy surfaces where you vary the key parameters of the model and explore how the transition probability varies with parameters.

(3) Second option: write a term paper on a research article on fundamental aspects of quantum mechanics relevant to chemical physics or physical chemistry. You are free to suggest the paper yourself, but here are a few examples:

(4) Third option: do some practical electronic structure calculations on a molecule of interest to you, perhaps in the context of your research. We can help you with access to production codes (well, our code anyway!). You will want to choose appropriate
methods to balance the accuracy of what you wish to compute against feasibility to make sure that you get some results in a few weeks!

(5) Proposal: Whenever you’re ready to start, write a short (< 1 page) plan for what you are going to do, and hand it to Rob or myself. Most likely we will approve it or suggest changes on the spot. You can do this any time starting immediately, but please not later than April 29.

(6) Assessment: This will come in two parts:
   (i) We will have short presentations during the week of finals so that everyone can learn a bit about you have been doing.
   (ii) There should also be a write-up of roughly 6-10 pages minimum that summarizes what you have done.