Fission in Exotic Nuclei Using DFT

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Contents

Chapter 1

Introduction

I don't really know how to make an abstract or something like that, and I know I'll have some other template to use when I actually start writing my thesis, but for the sake of having a place to put thoughts that may be useful later, here goes...

If you're looking for a central narrative with which to tie together your thesis, you could, of course, use the whole "making things faster" angle you've been playing so far. But I think a more enriching, exciting, and satisfying approach would be to emphasize that you are doing fission calculations for *rare* nuclei. That's cool because you work in a facility for *rare* isotopes! And it's just one of those things that is interesting and fashionable in the field in general right now. The introduction to the platinum-178 paper has a good discussion about the importance of trying to understand fission in regions of exotic isospin ratios, and how simpler models tend to be less reliable in those regions. That covers both the platinum and the r-process project motivations (at least partially), and oganesson is just interesting because of how heavy it is.

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It is an exciting time to study nuclear theory; for as we now enter the supercomputer age, we are able to implement the groundwork laid over the past several decades on modern, cutting-edge, high-performance computing centers. This allows

These advances in computing come simultaneously with advances in accelerator design and technology and other advances which allow experimental nuclear physics to reach far beyond what has been done before. For instance, the Facility for Rare

Isotope Beams (FRIB) at Michigan State University is projected to be able to nearly double the number of isotopes that can be produced synthetically. Together, state-of-the-art facilities for experiment and high-performance computing for theory are expected to lead to rapid advancement in our understanding of atomic nuclei.

One process which has always been a driver of nuclear physics is nuclear fission, the process by which a heavy nucleus decays into two smaller nuclei of approximately equal mass. Nuclear fission has been applied by humans in the fields of energy generation and national defense, and it has been predicted to play a major role in astrophysical environments such as neutron star mergers. There is currently a great deal of interest in understanding “rare” isotopes, or isotopes which are highly-unstable, in order to better understand such exotic phenomena as neutron star mergers, as well as to better identify physical properties which we can use to better understand the nuclei which we regularly encounter on Earth.

There are a couple of ways for a nucleus to fission. One way is by imparting some excitation energy to a fissile nucleus, such as by bombarding a nucleus with neutrons (neutron-induced fission) or by creating an excited nucleus as the decay product of another isotope (beta-delayed fission). Owing to the randomness of quantum mechanics, another possibilty is for a nucleus in its ground state to spontaneously tunnel through a potential barrier and then emerge to form two distinct fragment (spontaneous fission). This thesis will deal primarily/exclusively with the latter.

Theoretically, making predictions about fission is challenging because, thanks to the large number of particles involved and the complex collective interactions which take place when one system deforms and becomes two, fission calculations have an ”inextinguishable thirst for computing power,” as stated in [**?**]. Historically, most fission calculations that have been done were based on empirical formulas or phenomenological models, most notably the “microscopic-macroscopic” family of models based on Bohr’s liquid-drop model (to model the bulk properties of the nucleus) with Strutinsky shell corrections (to account for quantum mechanical shell effects). These microscopic-macroscopic (“micmac”) fission models are computationally fairly inexpensive, and can achieve quite satisfactory results. However, since the model is based on a phenomenological description of what is actually a quantum mechanical system, its predictive power is limited, and there is no clear way of making systematic improvements.

A more reliable approach would be to consider the individual nucleon states using some kind of quantum many-body method. For large systems with many, many particles, density functional theory (DFT) is a way to recast the Schrödinger equation involving $\sim$200 particles into a simpler problem involving only a few densities and currents (see section 2.0.2). With DFT as a way of calculating nuclear properties quantum-mechanically, one can then use these self-consistent solutions to predict fission properties, such as lifetimes and fragment yields. Fortuntately, a great deal of work has been done to achieve exactly this (see the review article [**?**]). Some of the ideas which are used were inspired by lessons learned from micmac and other, simpler models; others are unique to DFT. Our approach is described in detail in chapter 2.

Given the aforementioned recent interest in rare and exotic nuclei, we have applied our model to several exotic systems which undergo spontaneous fission in different regions of the nuclear chart. First in chapter 3 we discuss bimodal fission in the neutron-deficient isotope platinum-178, which until recently was expected to fission symmetrically. Then in chapter 4 we discuss cluster radioactivity in oganesson-294, the heaviest element ever produced by humans. In chapter 5 we move to the neutron-rich side of the nuclear chart to study ..., which are expected to play a major role in the astrophysical r-process. Finally, in chapter 6 we discuss the current state of the field, and, based on our experience, offer insights for guiding future developments in the field.

Chapter 2

Describing Fission Using Nuclear Density Functional Theory

Since nuclei are quantum mechanical systems, they can in principle be described using the Schrodinger equation. However, in practice one finds this type of description difficult or impossible, for two reasons:

- In order to use the Schrodinger equation, one needs to know how to describe the interaction between particles, such as between protons and neutrons. However, protons and neutrons are made up of quarks and gluons, which interact via the strong nuclear force. Consequently, an analytic expression for the nucleon-nucleon interaction analogous to the $\frac{1}{r}$ form of the Coulomb interaction is not available. Finding different mathematical expressions which can describe the interaction between nucleons continues to be an active area of research [**?**]

- Even when an interaction is known, nuclei are large systems made up of many protons and neutrons. Solving the Schrodinger equation directly quickly becomes computationally intractable as the number of nucleons increases.

2.0.1 Skyrme Interaction

2.0.2 Density Functional Theory

Kohn-Sham - Suppose you have the density of an interacting system. There exists a unique noninteracting system with the same density Then I believe HFB is put on top of that to do the variation part. I think I (approximately) get it now! - So just to make sure, what would DFT look like without HF/HFB? And HF/HFB without DFT?

2.1 Microscopic Description of Nuclear Fission

Should I describe these here, or in the sections when they actually get used?

2.1.1 Potential Energy Surfaces

Constrained HFB; map out many different constrained calculations and start to form a surface which resembles a topographical map

2.1.2 WKB Approximation

Adiabaticity: For fusion reactions, N,Z equilibrium reached in $\sim 10^{-21}$ seconds, then energy/thermal equilibrium in a similar time scale, then finally mass equilibrium in $\sim 10^{-19}$ - Yuri has a slide with these time scales from his talk Monday

Sort of an adiabatic approximation; useful because half-lives are long and therefore time-dependent approaches are impractical (they break down and/or become unstable or something after too many time steps, not to mention the amount of computing time). Wavefunction is assumed to be slowly-varying inside the potential barrier

Furthermore, TDHFB cannot tunnel

2.1.3 Langevin Dynamics

It has been shown (Jhilam and Nicolas' paper) that fission yields are fairly robust with respect to the dissipation strength

Chapter 3

Two fission modes in 178Pt

Bimodal fission in 178Pt?

3.0.1 Experiment

This project was done in conjunction with an experiment that was performed...

Elongation tends to minimize the Coulomb repulsion between fragments

Chapter 4

Cluster decay in 294Og

This was done in a 4D space consisting of the coordinates $(q_{20}, q_{22}, q_{30}, \lambda_2)$

We used 30 harmonic oscillator shells and 1500 states

4.0.1 Cluster Decay

Experimental instances of super-asymmetric fission: M. G. Itkis 1985, Z Phys A 320 - no assessment of the cause of highly-asymmetric fission, but likely related to 132Sn (there nuclei would tend to fission symmetrically, but with a slight bump around mass A=140-145) D. Rochmann Nucl Phys A 735 (2004) - driven by shell structure of lighter fragments I M Itkis, J Phys Conf Ser 515 (2014) 012008 - cluster radiation by another name

AKA Lead Radioactivity sometimes in the literature To predict cluster half-lives, some people take it as a very heavy alpha emission, and others a very asymmetric fission Warda looks at the N/Z ratio of known cluster emitters (or really of lead-208), and then extrapolates it out to SHEs. Thats how he decided which superheavies to compute PRC 86 (2012) 014322 Nucl Phys A 944 (2015) 442 (with Baran and others)

4.0.2 Synthesis of Og

They found 3 (and possibly 4) instances in the original Dubna run. Then there was a secondary run at Oak Ridge that was about the same: something like 3 alpha events and a possible fission event. (Another Og paper is being prepared (Nathan Brewer, et al), which has a similar decay chain but a shorter half-life (∼0.185 ms); Detected a 10.6 MeV recoil event, followed 78 microseconds later by a second decay event in the same pixel (∼140 MeV), which is a candidate for SF)

4.0.3 Competition with Alpha Decay

Recent efforts to synthesize superheavy elements (SHE) have successfully produced the isotope ^{294}Og, which has been confirmed via its alpha-decay chain. In both experiments, the researchers found evidence of alpha decay, but both also noted the possible observation of decay via spontaneous fission. This suggests the possibility that ^{294}Og might have a similar decay time with respect to both alpha-decay and spontaneous fission.

There has been an expectation (for some reason?) that cluster emission (known also in the literature as cluster radioactivity, lead radioactivity, cluster decay, heavy-particle radioactivity, ???) might play an important role in the fission of superheavy elements, suggesting that even for such large nuclei (where the Coulomb repulsion is strong), shell structure of the prefragments still drives the determination of the fragments.

[2, 10] - In this paper they propose changing/extending the concept of Heavy Particle Radioactivity or Cluster Radioactivity. Also they apply some model to HPR/CR in SHE.

“A larger number of observed spontaneous fission ac- tivities enabled the establishment of a global dependency of spontaneous fission half-lives (TSF) and the fissility of a nucleus, expressed by the ratio Z2/A which had been realized already by Seaborg [111] and also by Whitehouse and Galbraith [112]. The data, available at that time indicated for even-even nuclei an exponential dependence of the fission half-lives from Z2/A. From an extrapolation of the trend it was concluded, that a nucleus will become instantaneously unstable against nuclear fission at Z2/A 47, which was set in correspondence with a half-life of 1020 s. Interestingly, the heaviest nucleus reported to be synthesized so far, 294118 (294Og) [65], has a value Z2/A 47.36. The half-life is given as T1/2 =0.69+0.640.22 s. Up to now four decays, but no spontaneous fission was observed [65].” - from [6] - Og is anomolous in that it violates this extrapolated trend (as would, I am sure, most SHE).

Whether or not this PES is able to reasonably describe the CN experiments which so far have produced ^{294}Og is uncertain, because such large compound nucleus expectation energies as appear in experiment may have quite a large effect on the topology of the PES [8]

On the theory side, there have been several attempts to compute spontaneous fission half-lives and alpha-decay half-lives for many superheavy nuclei, and in many cases it is predicted that the two lifetimes will be comparable [2, 10, 18] [Zhang was an application of several universal CR and alpha decay models to the SHE, in order to see if the predictions, too, were universal]. These previous works have tended to rely on phenomenological models which have been tuned to smaller, more stable nuclei. Thus, it is difficult or impossible to assess these models' predictive power in the region of SHE. Thus, a goal of this work is to bring the full predictive framework of self-consistent nuclear density functional theory to bear on the problem of spontaneous fission in the SHE ^{294}Og. This approach is relatively young in the world of nuclear fission models, but it is already producing quality results for a variety of nuclei in different regions of the nuclear chart (see, for instance, [7, 15, 14, 9]). Some attempts in the region of SHE have already been made, using Skyrme and Gogny functionals in a 2D space [11, 5, 17, 3].

Within these models, spontaneous fission lifetimes tend to be considerably larger than alpha decay lifetimes, ranging from $\frac{\tau_{SF}}{\tau_\alpha} \approx 10^{-10}$ in [3] and [11] to $\frac{\tau_{SF}}{\tau_\alpha} \approx 10^{-20}$ in [17]. However, it was shown in [12] that pairing correlations treated as a dynamical variable can have a substantial impact on spontaneous fission lifetimes. That is explored in the case of ^{294}Og here.

4.1 Method

Our calculations were performed within the framework of nuclear density functional theory using Skyrme and Gogny energy density functionals. In the Skyrme case, the parameterization UNEDF1-HFB [16] was used, and pairing correlations were described using a density dependent pairing interaction. To assure convergence despite the high density of states, the DFT solver HFODD was used with 30 harmonic oscillator shells and 1500 states allowed in the calculation. Calculations were performed in a 4D collective space consisting of 3 shape coordinates, (q_{20}, q_{30}, q_{22}), and, given the importance of dynamic pairing fluctuations demonstrated in [12], λ_2. To demonstrate model independence, another set of calculations was performed using the Gogny energy density functional D1M in the two-dimensional collective space described by coordinates (q_{20}, q_{30}).

It is seen in many models that introducing triaxiality as a degree of freedom can often be energetically-favorable, sometimes lowering saddle points by as much as 3 MeV; however, dynamic calculations in which the collective inertia is considered together with the potential energy surface have found that dynamical pathways usually tend to tunnel through barriers rather than break axial symmetry. This competition was explored for SHE in [1], with the conclusion that triaxiality plays a fairly insignificant role in determining the half-life of elements below $Z = 120$. However, another recent paper (https://arxiv.org/abs/1803.04616v2) suggests that triaxiality might significantly lower the second barrier. Regardless, we included q_{22} in our calculations. It may also be the case that isotopes which are oblate-deformed in their ground state may pass through triaxial configurations on their way to greater elongations.

The basis of the model is the assumption that spontaneous fission can be treated such that the lifetime is proportional to e^{-P}, where P is the transmission probability through some barrier.

The collective inertia of the system was computed using the nonperturbative ATDHFB cranking approximation in the Skyrme case, and perturbative ATDHFB with cranking and perturbative GCM with cranking in the Gogny case [4]. The tunneling is described using the WKB approximation, in which the tunneling path $L(s)$ was computed by using the dynamic programming method to minimize the collective action

$$S(L) = \int_{s_{in}}^{s_{out}} \frac{1}{\hbar}\sqrt{2\mathcal{M}_{eff}\left(V_{eff}(s) - E_0\right)}ds \tag{4.1}$$

where $\mathcal{M}_{eff}$ is the effective inertia and V_{eff} the effective potential energy along $L(s)$. Following the formalism of [13], the half-life is computed via $T_{\frac{1}{2}} = \ln 2/nP$, where $n = 10^{20.38}s^{-1}$ is the number of assaults on the fission barrier per unit time and the penetration probability P is given by

$$P = (1 + exp[2S(L)])^{-1} \tag{4.2}$$

Finally, after computing the action at many points along the outer turning line, the final fragment yields were determined by evolving the system many times via Langevin dynamics, following the work done in [14].

Chapter 5

R-process

I'll say some stuff about r-process nuclei here

Chapter 6

Outlook

In this chapter, it would be great to talk to everyone you know (Witek, Samuel, Jhilam, Nicolas, Michal, and so on) to get a better feel for what kinds of issues need to be addressed next. You've already got sort of a rudimentary understanding (see your Google Keep note for starters), but it might be good to get some outsider perspective. This will be especially important as you start looking for postdocs, and *especially* especially if you end up looking for postdocs in nuclear theory, but not necessarily nuclear fission.

As I said in chapter 1, "Finally, in chapter 6 we discuss the current state of the field, and, based on our experience, offer insights for guiding future developments in the field."

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