FISSION IN EXOTIC NUCLEI USING DFT

By

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ABSTRACT

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This is my abstract.

Dedicated to I dunno

ACKNOWLEDGMENTS

I dunno who to acknowledge, either

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Introduction

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December 5, 2018

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.

It is an exciting time to study nuclear theory; major advances are now possible thanks to a groundwork lain of nuclear theory, paired with modern supercomputers fast enough for such complicated many-body problems to be solved.

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 dissertation 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 ~200 particles into a simpler problem involving only a few densities and currents (see section 2.1.1). 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.

The challenge, now, is to do these calculations cheaply. In every theoretical calculation, one must ask oneself "What approximations can I safely make?" and "What are the important degrees of freedom for this problem?" One may also reduce the total time-to-answer via improvements to the computational workflow itself, such as better file handling and parallelization.

1.1 Goals of the project

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

(Nicolas gave a good annotated presentation in 2017 that describes some of the philosophy, as well as some of the outstanding challenges of spontaneous fission in an adiabatic framework: `https://t2.lanl.gov/fiesta2017/school/Schunck_NotesSlides.pdf`)

Spontaneous nuclear fission is a type of quantum tunneling; consequently, it should be described using quantum mechanics.

2.1 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.

2.1.1 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?

Rather than find the density of a system of interacting particles (which can be extremely complicated - as one particle moves, the force it exerts on neighboring particles causes them to move, which will in turn change the magnitude and direction of the net force acting on the original particle, and so on until an equilibrium configuration, if it exists, can be attained), Kohn-Sham allows us to find an equivalent density of fictional non-interacting particles. That is, instead of particles moving in a field generated by many interdependent neighboring particles, one may think of non-interacting particles moving about a mean-field, which is essentially an averaging over all other particles.

Together, the Hohenberg-Kohn theorems state that if one is able to find the true ground state density, regardless of where it comes from, then there exists a unique functional of the density which gives the ground state energy of the system. However, HK do not specify how this functional is to be obtained.

For a variety of reasons/complications, pure Kohn-Sham is not used in nuclear physics; however; in the spirit, we oftentimes switch to a representation involving densities (which are directly and exactly attainable from a many-body wavefunction) and energy density functionals (which are not known exactly). (Wait, but then what is the point of converting to densities? Why not just leave them as wavefunctions? Or maybe we do, but this representation just makes the math look nicer for papers)

2.1.2 Skyrme Interaction

In DFT there is proof of existence, but no recipe for finding the energy density functional corresponding to a given system. $\Rightarrow$ Is it true to say I'm actually using DFT? Or just SCMF via HFB? ...is only as good as its energy density functional. In principle the Kohn-Sham formulation of quantum mechanics is exact

We use DFT to recast many-body QM into something tractable (depending on ρ and κ, not Ψ) We use Skyrme as our approximate interaction (with coefficients fitted to data) We use HF/HF+BCS/HFB to solve the Kohn-Sham equations by varying with respect to the configuration (in this case, ρ and κ) (? This one I'm not as sure about)

The energy density means:

$$E = \int d^3\vec{r} \sum_{t=0,1} \mathcal{H}_t \tag{2.1}$$

where $t = 0(1)$ refers to isoscalar(isovector) energy densities. The total energy density is a sum of both time-even and time-odd terms:

$$\mathcal{H}_t = \mathcal{H}_t^{even} + \mathcal{H}_t^{odd} \tag{2.2}$$

$$\mathcal{H}_t^{even} = C_t^\rho \rho_t^2 + C_t^{\Delta\rho} \rho_t \Delta\rho_t + C_t^\tau \rho_t \tau_t + C_t^J \mathsf{J}_t^2 + C_t^{\nabla J} \rho_t \nabla \cdot \vec{J}_t \tag{2.3}$$

$$\mathcal{H}_t^{odd} = C_t^s \vec{s}_t^2 + C_t^{\Delta s} \vec{s}_t \Delta \vec{s}_t + C_t^T \vec{s}_t \cdot \vec{T}_t + C_t^j \vec{j}_t^2 + C_t^{\nabla j} \vec{s}_t \cdot (\nabla \times \vec{j}_t) \tag{2.4}$$

where τ_t is the kinetic energy density; J_t is the spin current density, with vector part given by $\vec{J}_{\kappa,t} = \sum_{\mu\nu} \epsilon_{\mu\nu\kappa} \mathsf{J}_{\mu\nu,t}$; $\vec{s}_t$ is the spin density, $\vec{T}_t$ is the spin kinetic density; and $\vec{j}_t$ is the momentum density (to see how these are related to ρ_t, see, e.g., [6]). Note that $\mathcal{H}_t^{even}$ depends only on time-even densities (and likewise for $\mathcal{H}_t^{odd}$).

2.2 Microscopic Description of Nuclear Fission

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

With the nuclear physics somewhat under control, we now move onto the problem of using it to actually describe fission. For induced-fission, time-dependent density functional theory (TDDFT) allows one to calculate the time-evolution of a nucleus starting from some deformed initial configuration. So far, though, this approach has not been able to estimate a full yield for a fissioning nucleus; rather, the system propogates deterministically to a single scissioned configuration. Furthermore, and especially important for the case of spontaneous fission, the time-dependent approach does not allow for tunneling (why not?).

Nuclear fission is the fundamental physical process by which a heavy nucleus decays to two smaller nuclei with approximately equal masses, and a proper understanding of fission is critical for applications . It is a highly-collective process involving all the constituent nucleons of the system, and thus since its discovery it has been described via large shape deformations of an otherwise spherical “drop” of nucleons. In this framework, which is formalized by the adiabatic approximation, it falls upon theorists to describe many different nuclear shapes. In principle, one could describe any three-dimensional shape using an infinite basis such as the multipole expansion which is often encountered in eletrodynamics; however, for practical computations one must used a truncated set of only a few multipole moments (or, more generally, collective coordinates). Thus, an important challenge for researchers is to select the most relevant collective coordinates, ideally while demonstrating that others can be safely neglected.

Recently in [17], an approach based on this assumption was used to compute fragment yields from a potential energy surface (PES) that was computed self-consistently, using the WKB approximation to describe the tunneling and Langevin dynamics to describe post-scission dissipation. Now we test robustness of these results by exploring the impact of the energy density functional, the size of the collective space, and the calculation of the collective inertia on fragment yields.

2.2.1 Potential Energy Surfaces

Constrained HFB; map out many different constrained calculations and start to form a surface which resembles a topographical map. How do you decide which collective coordinates to use? Including pairing...

Physically, a nucleus can be thought of as a jumble of particles, each bouncing around in a potential well determined by the surrounding nucleons. Qunatum mechanics forbids us from determining the particle trajectories exactly; however, it allows us to estimate the probabilities of certain outcomes. In the case of fission, the most common approach has us thinking of nucleons grouping together collectively in a way which resembles a liquid drop (footnote: this idea was first proposed by Niels Bohr, I believe, and has proven to be a very fruitful way to describe fission). The collective shape is constrained to nearly-spherical shapes by a potential barrier; however, being a quantum mechanical system there is some nonzero tunneling probability, or a probability that the barrier will be penetrated, and the collective shape will stretch beyond the size fixed by the barrier. When this happens, the nucleus may remain in a long-term elongated state (called a fission isomer), or it may continue to deform until it separates into two fragments.

2.2.2 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

2.2.3 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

Fission is most well-studied in the region of the actinides (Z=90 to Z=103), as many naturally-occurring isotopes in this region are fissile. Within this region, there is a characteristic tendency for fission fragment yields to be asymmetric (that is, one light fragment and one heavy fragment), with the heavy peak centered around $A \approx 140$. This has been understood as a manifestation of nuclear shell structure in the prefragments: doubly-magic ^{132}Sn drives the nucleus towards scission, and once the neck nucleons are divided up between the two fragments, we end up with the heavy fragment A=140 peak. As one moves to the lower-Z actinides, however, this tendency becomes less and less pronounced as yields tend to become more symmetric. Below thorium, it was generally believed (though mostly not tested) that yields would continue to be symmetric as there was no doubly-magic nucleus candidate that could reasonably be expected to drive the system toward asymmetry as there is with actinides.

However, it was reported in a paper published in 20?? [**?**] that neutron-deficient ^{180}Hg undergoes beta-delayed fission to produce two fragments of unequal mass. This finding triggered a flurry of theoretical papers hoping to describe this new and unexpected phenomenon.

A follow-up experiment was performed in 20?? [**?**] investigating spontaneous fission of ^{178}Pt, which differs from ^{180}Hg by 2 protons. This system was studied at various excitation energies and found to fission pretty consistently with a bimodal pattern. Of the nuclei which

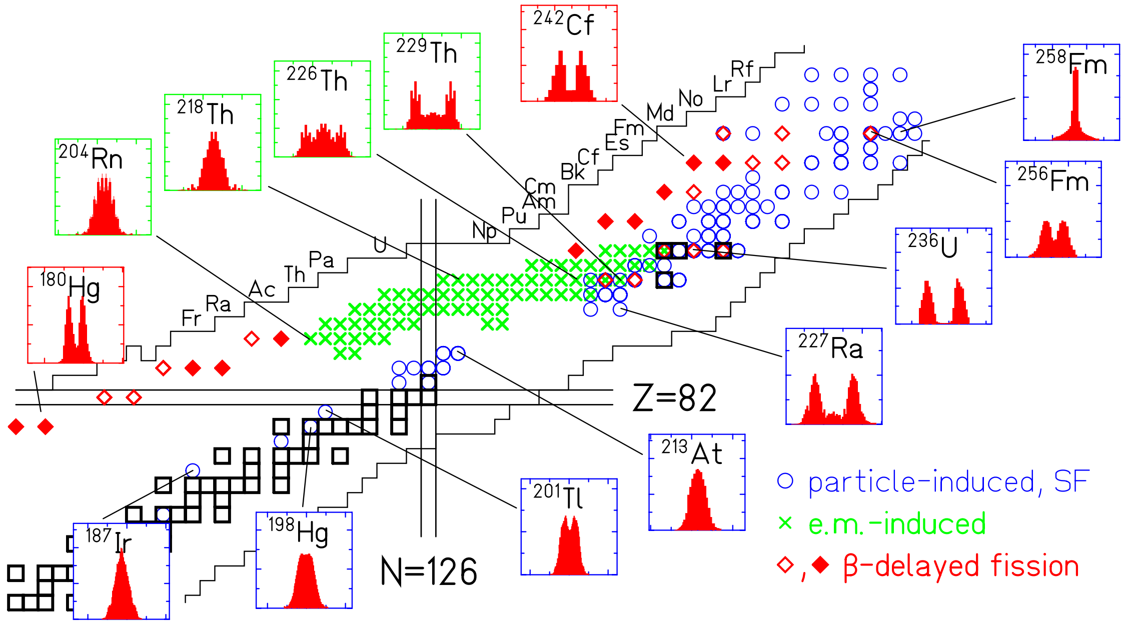

Figure 3.1: Fragment yields for several nuclei ranging from actinides, where primary fission yields tend to be asymmetric, down to near-thorium, where yields become more symmetric except in the region near neutron deficient ^{180}Hg. Figure from [2].

underwent spontaneous fission, roughly 1/3 were found to fission symmetrically while the other 2/3 fissioned asymmetrically with a light-to-heavy mass ratio of approximately 80/98 (Is that the correct ratio?). Furthermore, it was observed that symmetric fragments tended to have higher kinetic energies than non-symmetric fragments.

Elongation tends to minimize the Coulomb repulsion between fragments

Why is there a region of symmetric fission below thorium?

Chapter 4

Cluster decay in 294Og

4.1 Introduction

An exciting frontier in nuclear physics is the region of superheavy nuclei ($Z \geq 104$). The latest experiments are able to push the boundaries of the nuclear chart all the way to Z=118, and new ideas are being developed to increase production and improve measurements of superheavy elements [**?**, **?**]. Due to the large number of nucleons, these nuclei push the limits of our nuclear structure models and are expected to highlight new aspects and phenomena of nuclear physics. Spontaneous fission, for example, will likely play an important role in governing the lifetimes of many of these new systems. Fission of superheavy elements may also play an important role in the astrophysical r-process, by placing an endpoint on neutron capture and starting fission cycling (see, e.g., [8]).

As these pioneering experimental efforts are made, theory plays a critical role by guiding and interpreting the results of those experiments, as well as by filling in gaps where experiment cannot reach. However, in these exotic regions it is especially important to use only the very best and most reliable predictive models. Recently, a great deal of work has been invested in building self-consistent microscopic models of spontaneous fission which are able to predict, for instance, half-lives and fragment yields [16, 15, 17, 18].

However, this success comes at a cost. In the adiabatic approaches that are often invoked to describe spontaneous fission, fission is described as a tunneling through a potential barrier in a multidimensional space of collective nuclear shape coordinates. Due to the large computational cost associated with calculations (their "inextinguishable thirst for computing power," as stated in [?]), this barrier is approximated using five or fewer shape coordinates in phenomenological microscopic-macroscopic models, and even fewer in mean-field approaches.

Of course, it is well-understood that some physics may be obscured in a limited collective space (see [7]). Thus, one's choice of collective coordinates is dependent on what physics are deemed important or relevant, and which aspects can be safely neglected. In mean-field models, the collective coordinates are typically chosen to be leading order terms in the shape multipole expansion: axial quadrupole moment, triaxial quadrupole moment, and axial octupole moment. Additionally, it was shown in a previous work [15] that pairing correlations have a strong impact on the half-lives calculated via action minimization, and should be taken as a collective coordinate equal in importance to multipole moments or other shape-based collective coordinates.

In the following sections we try to understand the role of the collective space on fission yield predictions. In section **??** we describe the microscopic framework used here to calculate fragment yields, and then in section **??** the model is applied to the superheavy element ^{294}Og, which is the heaviest element ever produced by humans. The paper then concludes with analysis and discussion of the results in section **??**.

4.2 ^{294}Og

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.

While some authors [cite] have predicted that fission in the superheavies will proceed as with the actinides (that is, driven by the shell formation of ^{132}Sn in one of the prefragment) our calulations predict that the dominant fission mode will be highly-asymmetric and driven by ^{208}Pb (sometimes referred to in the literature as cluster emission).

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.

[3, 13] - 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 activities enabled the establishment of a global dependency of spontaneous fission half-lives (T_{SF}) and the fissility of a nucleus, expressed by the ratio Z^2/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 Z^2/A. From an extrapolation of the trend it was concluded, that a nucleus will become instantaneously unstable against nuclear fission at $Z^2/A \approx 47$, which was set in correspondence with a half-life of $\approx 10{-}20$ s. Interestingly, the heaviest nucleus reported to be synthesized so far, ^{294}118 (^{294}Og) [65], has a value $Z^2/A \approx 47.36$. The half-life is given as $T_{1/2} = 0.69 + 0.640.22$ s. Up to now four α decays, but no spontaneous fission was observed [65]." - from [9] - 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 [11]

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 [3, 13, 21] [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, [10, 18, 17, 12]). Some attempts in the region of SHE have already been made, using Skyrme and Gogny functionals in a 2D space [14, 8, 20, 4].

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 [4] and [14] to $\frac{\tau_{SF}}{\tau_\alpha} \approx 10^{-20}$ in [20]. However, it was shown in [15] 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.

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

A criticism that is sometimes leveraged against self-consistent mean-field-based approaches to fission is that, due to the large computational cost associated with calculations, typically only one or two collective coordinates are used. This is in contrast to microscopic-macroscopic methods, where up to five collective coordinates are often used. Those who use SCMF methods assert that the dominant characteristics of the nuclear collective motion necessary for understanding fission can be sufficiently described using perhaps the axial quadrupole moment and maybe one other multipole moment which depends on the specific system, often the axial octupole moment or triaxial quadrupole moment. Of course, it is well-understood that some physics may be obscured in a limited collective space (see [7]). Thus, one's choice of collective coordinates is dependent on what physics are deemed important or relevant, and which aspects can be safely neglected.

However, although various attempts have been made to demonstrate the validity of this assumption, our work represents the first published instance of a 4D potential energy surface calculated self-consistently. Furthermore, given the recent demonstration of the importance of pairing correlations as a collective "coordinate" of the system, ours will feature pairing as part of the collective space, and its impact compared to other collective coordinates will be evaluated.

We used 30 harmonic oscillator shells and 1500 states

4.2.1 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. That’s how he decided which superheavies to compute PRC 86 (2012) 014322 Nucl Phys A 944 (2015) 442 (with Baran and others)

4.2.2 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 ($\sim$0.185 ms); Detected a 10.6 MeV recoil event, followed 78 microseconds later by a second decay event in the same pixel ($\sim$140 MeV), which is a candidate for SF)

4.2.3 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.

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4.3 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 [19] 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 [15], 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 [5]. 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 [16], 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 [17].

4.4 Langevin dynamics

Chapter 5

R-process

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

Fission inputs to r-process network calculations

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."

We definitely need a better handle on the inertia. The perturbative inertia is easy to compute, but not terribly reliable. The non-perturbative inertia can certainly do better, but as it is computed now (using finite differences) it is subject to numerical artifacts and instabilities (dependent on the level of convergence of the individual densities, the coefficient mutlipliers, different basis sizes) and actual physics, such as level crossings which manifest in projections from a higher-dimensional space.

UNEDF1 seems to underestimate fission barrier heights (artificial though the concept may be; the main impact is probably that lifetimes are underestimated). It also turns out to be a headache to work with, making convergence quite a challenge sometimes (any cases in particular, like for highly-deformed or heavy or octupole-deformed nuclei or something?).

Better functionals might hope to better capture the physics, and one can hope they are easier to work with.

APPENDIX

Appendix

Temperature-Dependent ATDHFB Collective Inertia

Everything which was shown in this dissertation assumed that the system was maintained at temperature $T = 0$ and the nucleus behaved as a superfluid below the Fermi surface. However, in many environments (such as a neutron star merger or a nuclear blast) there may be quite a bit of excitation energy imparted to the system, which would raise the temperature above the Fermi surface. In this case, pairs may be broken and the topology of the potential energy surface may change (see, for instance, [10]). In this case, the collective inertia of the system is changed, too, as shown below.

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