My PhD Thesis

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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.

Chapter 2

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. How do you decide which collective coordinates to use? Including pairing...

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

Why is there a region of symmetric fission below thorium?

Chapter 4

Cluster decay in 294Og

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.

[**?**, **?**] - 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 [?] - 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 [?]

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 [?, ?, ?] [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, [?, ?, ?, ?]). Some attempts in the region of SHE have already been made, using Skyrme and Gogny functionals in a 2D space [?, ?, ?, ?].

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

4.0.1 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

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 [?] was used, and pairing correlations were described using a density dependent pairing interaction. Calculations are 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 [?], 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}).

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 [?]. 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 [?], 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 [?].

Chapter 5

R-process

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

Fission inputs to r-process network calculations

Bibliography