EXCITING DISSERTATION TITLE

By

Your Name Here

A DISSERTATION

Submitted to
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ABSTRACT

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I dedicate this work to the Opossum and his noble pursuit of snacks.

ACKNOWLEDGMENTS

Una Salus Victis Nullam Sperare Salutem.

PREFACE

This is my preface. remarks remarks remarks

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Chapter 1. Introduction

Fission was first observed accidentally by Fermi, when he bombarded uranium with neutrons in an attempt to create heavier nuclei. The first observation of fission was, therefore, neutron induced. Since then, fission has been widely studied with a number of entrance channels, including γ- and light-particle-induced [cite], and, recently, neutrino-induced [cite]. Spontaneous fission is markedly different from these, because it is not induced by particle interactions.

To understand the various observable quantities present in fission, we consider a single fission event chronologically. In induced fission, the first quantity is the cross section, which measures how likely a fission event is to be induced. For a review of the state of the field, see [refs]; since this work primarily studies SF, we will not dwell any longer on the cross section. [change if ν-fission paper is out]

For SF, then, the starting point is a static nucleus, sitting in its ground state. Induced fission will use many of the same tools, except assuming an excited state of a compound nucleus (i.e. an equilibrated nucleus that has no memory of how it was formed). The nucleus deforms, elongating in a (commonly asymmetric) manner, until it eventually splits, called scission (notice that this description ignores second- and third-chance fission, in which neutron(s) are emitted pre-scission). The timescale of this splitting varies greatly: some nuclei [example 1] live for $\sim 10^8$ seconds, while others last for [lower bound]. The timescale is only important for SF, and is called the SF lifetime (induced fission I think you can't measure this timescale...?).

Typically, two fragments are formed, although three fragments have been observed rarely [cite]. The fragments are determined probabilistically, and form a distribution in both Z and

A, called the primary fission fragment distribution [cite examples]. Typically, these yields are not observed directly - the fragments begin to decay roughly 10^{-18} seconds after the nucleus splits, see Ref. [2] - but are instead inferred afterwards [find lit for this].

At this point, the fragments are highly excited, and are accelerated away from each other by the Coulomb force. The energy in these fragments is called the total kinetic energy [find good source for how it's measured]. As the fragments accelerate, they de-excite via neutron and γ emission [saw many good papers on this]. The emitted particles can be measured, leading to neutron multiplicities [define], photon energies, and, a subject of much interest recently, photon angular momentum [cite stuff] correlations. I think this is also how one backs out the primary fragment yields?

After the fragments de-excite as much as possible, the remaining fragments are still (typically) unstable. On long timescales, these nuclei undergo β decay, moving towards stability. This spectrum can be measured, and the remaining stable nuclei form a distribution known as the cumulative fission yields. [comment on difficulty measuring data at this timescale]

All told, a unified description of fission would require a model that is descriptive from $10^{-18} - 10^{8}$ s. Rather than undertake such an absurd task, different timescales are treated using different models. This divide is not fixed, but a typical divide can be seen in Fig. 2 of Ref. [2]: the entrance channel, collective motion leading to primary fragment yields, statistical particle emission, and eventual β decay are each treated separately. This work focuses solely on the collective motion leading to the primary fragment yields; for a review of the other processes, see [cite - maybe just Ref. [2] again].

There are essentially two models used to describe this collective motion. blah blah blah mic-mac and DFT

Start with how we do things in fission studies (ie dft $\rightarrow$ pyneb), then go to discrepancies between models (multimodal paper), then discuss emulation strategies for dft

Things to discuss about fission:

- Brief historical intro
- Different stages/timescales in fission, and observable quantities at each stage
- Discussion on primary fragment yields and SF lifetimes (maybe as part of the previous section)
- Astrophysical motivation? Other scientific use cases for primary fission observables? Connection to other areas of nuclear structure/reactions theory?

Next section: methods for computing fission observables

- Brief outline of DFT. Don't see a reason to describe all the gory details here, not even things like the EDF used. Make sure to include inertia tensor, not just PES
- Discussion of tunneling - maybe belongs prior to DFT discussion? Tunneling happens with or without DFT, after all
- Somewhere here I need to bring up other approaches. Main one is mic-mac plus Langevin; not sure how to work that in. Since we can do Langevin on DFT PESs, maybe a point of comparison there...? Tricky, b/c it could end up looking like I'm saying their work is improper, somehow. I see: Langevin belongs in next section. It doesn't get tunneling path at all - just the yields themselves. With mic-mac PESs, point out that LAP hasn't been computed there (yet!)
- Previous algorithms used for tunneling paths

- Pyneb
- Results (comparison with previous algorithms, any runtime information at all)

Next section: multimodal paper

- Maybe here worth discussing different fragment yield models? To point out that different methods exist, and that they make different predictions
- Discuss fragment yield calculations here, once we've arrived at exit point (doesn't really make sense in tunneling discussion)
- Explain meaningful differences between the EDFs we consider: finite-range vs point-like, what they were fit to
- Compare results in 2d for Fm isotopes. Superheavy discussion doesn't really add to the discussion? Can just refer to paper
- Discuss different sets of collective coordinates somewhere. Include axial/triaxial coordinates, lit review, etc
- Compare 3D results to 2d results for 254Fm, 258Fm

Next section: emulators

- Need astrophysics motivation before NN paper. Either in intro, or briefly here (or both)
- Black-box emulation as a strategy for computing PESs and inertias
- Results for exit points and lifetimes from above method

- Insensitivity to network size? Doesn't really add much; maybe just a comment on it and leave it to the original paper

Next section: intrusive emulators (for SCMF in general)

- Somewhere above, motivate Bayesian UQ - perhaps in section on multimodal paper
- Discuss on a high-level the basis expansion method for solving HFB equations, and why we use it
- Example with BGG equation, to show why it's annoying computationally, what to do about it, and how that helps
- High-level description for Skyrme EDFs, repeating the same thing (could possibly get away with no eqns in this section)

Chapter 2. Density Functional Theory

Fission occurs in heavy nuclei ($A \gtrsim$ whatever). Although ab-initio approaches to nuclear structure have made much progress in the past decade, such methods struggle to reach past the medium-mass region of the nuclear chart. Similarly, shell-model approaches cap out at [some other value]. The only [GCM and other beyond-mean-field methods exist][check this] approach based on an effective nucleon-nucleon interaction that can reach heavy regions of the chart is (nuclear) density functional theory (DFT). It has been used in [insert literature review here] for nuclear structure and dynamics, and blah blah blah. DFT is the primary underlying methodology used throughout this work. As such, we will detour from the fission discussion to provide a (brief) overview.

2.1 The HFB Equations

The HFB equations have been derived in many works [list some], and many of their properties have been explored [elsewhere]. Here, we will simply summarize the key features. It is also worth noting that DFT can be done at the Hartree-Fock level, and many works have studied pairing only at the BCS level; throughout, we will pursue full HFB.

HFB can first be understood supposing we start with a second-quantized interaction, composed of creation and annihilation operators $a_i^\dagger$, a_j: [check indices]

$$H = \sum_{ij} t_{ij} a_i^\dagger a_j + \sum_{ijkl} \bar{v}_{ijkl} a_i^\dagger a_j^\dagger a_k a_l + \cdots \tag{2.1}$$

These operators obey the anticommutation rules $\{a_i, a_j^\dagger\} = \delta_{ij}$, $\{a_i, a_j\} = 0$. Rather than computing the full spectrum of the Hamiltonian, we use the variational principle with a

suitable wavefunction ansatz to approximately determine the ground state energy. [want to say that wavefunctions that are written using creation/annihilation operators are simple to write out equations of motion for]

A number of useful variational wavefunctions exist. The independent-particle picture is an accurate depiction of nuclear motion, hence the success of shell-model-type approaches. As such, an appropriate wavefunction is the Slater determinant, which lets describes nucleons moving independently within a mean field. The key difference from shell-model approaches [be careful with who I attribute things to] is that the mean field is determined self-consistently via the variational principle.

It is well established that pairing effects are important for [list things it helps with]. The simplicity of the single-particle picture can be retained, even while capturing much of the pairing effects [correlations?], by instead discussing the independent *quasi*-particle picture. This leads to the HFB equations. In mathematical terms, the HFB wavefunction $|\mathrm{HFB}\rangle$ is a single Slater determinant, expressed in terms of quasiparticle operators $\alpha_i^\dagger, \alpha_j$ via the Boguliubov transformation:

$$\alpha_k = \sum_n (U_{nk}^* a_n + V_{nk}^* a_n^\dagger), \quad \alpha_k^\dagger = \sum_n (V_{nk} a_n + U_{nk} a_n^\dagger). \tag{2.2}$$

For this wavefunction, the ground-state energy can be computed straightforwardly:

$$E_{\mathrm{HFB}} = \frac{\langle \mathrm{HFB}|H|\mathrm{HFB}\rangle}{\langle \mathrm{HFB}|\mathrm{HFB}\rangle} = \mathrm{tr}\left[\left(t + \frac{1}{2}\Gamma\right)\rho\right] - \frac{1}{2}\mathrm{tr}[\Delta\kappa^*]. \tag{2.3}$$

The particle, ρ, and pairing, κ, one-body densities are defined as [indices]

$$\rho_{ij} = (V^* V^T)_{ij}, \quad \kappa_{ij} = (V^* U^T)_{ij}, \tag{2.4}$$

and the mean-field potential and pairing field are

$$\Gamma_{ik} \equiv \frac{\delta E}{\delta \rho_{ji}} = \bar{v}_{ijkl}\rho_{lj}, \quad \Delta_{ij} \equiv \frac{\delta E}{\delta \kappa^*_{ji}} = \frac{1}{2}\bar{v}_{ijkl}\kappa_{kl}. \tag{2.5}$$

Note that ρ and κ are not independent variables, but the variational derivatives treat them independently.

The HFB equations can be derived following e.g. Refs [whatever]. The result is the self-consistent eigenvalue problem

$$\mathcal{H}\begin{pmatrix} U \\ V \end{pmatrix} = D\begin{pmatrix} U \\ V \end{pmatrix}, \quad \mathcal{H} = \begin{pmatrix} h & \Delta \\ -\Delta^* & -h^* \end{pmatrix}. \tag{2.6}$$

The matrix $\mathcal{H}$ is called the HFB matrix. Note that, even for a standard two-body interaction, $\mathcal{H} = \mathcal{H}[\rho, \kappa]$. Therefore, this problem must be solved self-consistently, which is typically done via some iteration scheme.

In position space, the total energy E_{HFB} can be written as an integral over the energy density,

$$E_{\mathrm{HFB}}[\rho, \kappa] = \int d^3r\, \mathcal{E}[\rho(\boldsymbol{r}), \kappa(\boldsymbol{r})]. \tag{2.7}$$

$\mathcal{E}$ is called the energy density functional (EDF) [check that it's not E_{HFB} that's the functional - Ref. [1] seems to agree with my vocabulary]. Via the Hohenberg-Kohn theorems, there is a

correspondence between the exact many-body wavefunction and the ground-state density of the system [cite]. That is, there exists an EDF for which ρ describes the true nuclear ground state. Therefore, while historically work has focused on many-body interactions (as will be seen with the Gogny interaction), much recent work has instead gone into determining the nuclear EDF.

2.2 The Energy Density Functional

Quite generically, the EDF can be written as

$$\mathcal{E}(\boldsymbol{r}) = \mathcal{E}_{\text{kin}} + \mathcal{E}_{\text{Coul}} + \mathcal{E}_{\text{ph}} + \mathcal{E}_{\text{pp}}, \tag{2.8}$$

although different authors organize the terms differently. These terms are composed of local densities. Such densities can be categorized based on their behavior under time reversal symmetry, although $\mathcal{E}$ is even under time-reversal symmetry. For the ground state of an even-even nucleus, the time-odd densities vanish [citation for this], so we will only introduce the time-even densities.

The various densities ρ_q, τ_q, and $J_{\mu\nu,q}$ are derived from the one-body density matrix, written in position space as

$$\rho_q(\boldsymbol{r}\sigma, \boldsymbol{r}'\sigma') = \sum_k V_{kq}(\boldsymbol{r}\sigma) V^*_{kq}(\boldsymbol{r}'\sigma'). \tag{2.9}$$

The index q labels the nucleon species ($q = n, p$) and σ, σ' are the spin indices. Unlike in Hartree-Fock theory, single-particle states have partial occupancies, i.e. the norm of the lower components of the eigenvectors, $N_{kq} = \int d^3r \sum_\sigma |V_{kq}(\boldsymbol{r}\sigma)|^2$, can take on any value

between 0 and 1. Therefore, the sum over k is over all states (at least, all those allowed by the pairing regularization procedure - see e.g. Ref. [10] for a discussion with a zero-range pairing interaction). The spin dependence of the particle density is decomposed as

$$\rho_q(\boldsymbol{r}\sigma, \boldsymbol{r}'\sigma') = \frac{1}{2}\rho_q(\boldsymbol{r}, \boldsymbol{r}')\delta_{\sigma\sigma'} + \frac{1}{2}\sum_i (\sigma|\sigma_i|\sigma')\rho_{i,q}(\boldsymbol{r}, \boldsymbol{r}'), \tag{2.10}$$

where the σ_i are the usual Pauli matrices. The local particle density $\rho_q(\boldsymbol{r})$, kinetic energy density $\tau_q(\boldsymbol{r})$, and spin-current density $J_{\mu\nu,q}(\boldsymbol{r})$ are then defined as

$$\rho_q(\boldsymbol{r}) = \rho_q(\boldsymbol{r}, \boldsymbol{r}),\ \tau_q(\boldsymbol{r}) = \nabla_{\boldsymbol{r}}\nabla_{\boldsymbol{r}'}\rho_q(\boldsymbol{r}, \boldsymbol{r}')|_{\boldsymbol{r}'=\boldsymbol{r}},\ J_{\mu\nu,q}(\boldsymbol{r}) = \frac{1}{2i}(\nabla_\mu - \nabla'_\mu)\rho_{\nu,q}(\boldsymbol{r}, \boldsymbol{r}')|_{\boldsymbol{r}'=\boldsymbol{r}}. \tag{2.11}$$

[probably want to provide intuition on how these terms commonly appear - e.g. J corresponds to the spin-orbit thing we're familiar with] These densities have analogues in the particle-particle channel, written in terms of the pairing density matrix

$$\tilde{\rho}_q(\boldsymbol{r}\sigma, \boldsymbol{r}'\sigma') = -\sum_k V_{kq}(\boldsymbol{r}\sigma)U^*_{kq}(\boldsymbol{r}'\sigma'), \tag{2.12}$$

as discussed in Ref. [4]. However, as commonly-used pairing EDFs $\mathcal{E}_{\rm pp}$ ignore these densities, they will not be expanded upon here. [relate $\tilde{\rho}$ and κ?]

The kinetic energy density is simply

$$\mathcal{E}_{\rm kin} = \sum_q \frac{\hbar^2}{2m_q}\tau_q(\boldsymbol{r}), \tag{2.13}$$

with m_q the nucleon mass. Commonly, one sets $\hbar^2/(2m_q) = 20.73553$ [units], as in [unedf1

calibration]. The Coulomb energy density contains the direct and exchange terms,

$$\mathcal{E}_{\text{Coul}} \equiv \mathcal{E}^{D}_{\text{Coul}} + \mathcal{E}^{E}_{\text{Coul}}. \tag{2.14}$$

[want nice reference for this] The direct term depends on $\rho_p(\boldsymbol{r})$, and is simple to evaluate directly:

$$\mathcal{E}^{D}_{\text{Coul}} = \frac{e^2}{2}\rho_p(\boldsymbol{r}) \int d^3r' \, \frac{\rho_p(\boldsymbol{r'})}{|\boldsymbol{r} - \boldsymbol{r'}|}, \tag{2.15}$$

where e is the electron charge. Numerical techniques for evaluating this integral have been discussed in Ref. [10] [and others]. The exchange term, on the other hand, is [9]

$$\mathcal{E}^{E}_{\text{Coul}}(\boldsymbol{r}) = -\frac{e^2}{2} \sum_{kk'\sigma\sigma'} V_{kp}(\boldsymbol{r}\sigma) V^{*}_{k'p}(\boldsymbol{r}\sigma) \int d^3r' \, \frac{V^{*}_{kp}(\boldsymbol{r'}\sigma') V_{k'p}(\boldsymbol{r'}\sigma')}{|\boldsymbol{r} - \boldsymbol{r'}|}, \tag{2.16}$$

which depends instead on $\rho_p(\boldsymbol{r}\sigma, \boldsymbol{r'}\sigma')$. While some works evaluate this exactly, see e.g. [hfbtho v4 and others], it is numerically expensive. Instead, one commonly uses the Slater approximation to write

$$\mathcal{E}^{E}_{\text{Coul}}(\boldsymbol{r}) \approx -\frac{3}{4}e^2 \left(\frac{3}{\pi}\right)^{1/3} \rho_p^{4/3}(\boldsymbol{r}), \tag{2.17}$$

and extensions depending on only $\rho_p(\boldsymbol{r})$ have been discussed in e.g. Ref. [6]. [probably should add discussion about impact of this approximation here]

Nuclear physics is contained solely in the particle-hole and particle-particle terms, $\mathcal{E}_{\text{ph}}$ and $\mathcal{E}_{\text{pp}}$, respectively. This separation is somewhat artificial, as, while $\mathcal{E}_{\text{ph}}$ depends only on ρ_q and its derivatives, $\mathcal{E}_{\text{pp}}$ depends both on ρ_q and $\tilde{\rho}_q$. Over the last few decades, many

EDFs have been developed [list useful references]. The most common EDFs are the Skyrme [cite] and Gogny [3], both of which have a large number of parameterizations that have been developed. Further, recent efforts to go beyond these forms have included [whatever e.g. Fayans]. For a recent overview, see e.g. [list references]. While many of the techniques developed throughout this thesis apply quite generally, we will focus next on the Skyrme- and Gogny-type EDFs.

2.2.1 The Skyrme EDF

The Skyrme EDF [something something history of it] is based on the density matrix expansion. It is motivated by the short range of the nucleon-nucleon interaction, which suggests that the full one-body density matrix $\rho(\boldsymbol{r}, \boldsymbol{r'})$ can be expanded about $\boldsymbol{r} - \boldsymbol{r'} \approx 0$, see e.g. Ref. [1]. In the particle-hole channel, the (time-even) nuclear part of the EDF is commonly written in the form [5]

$$\mathcal{E}_{\mathrm{Sk}}(\boldsymbol{r}) = \sum_{t=0,1} \chi_t(\boldsymbol{r}), \tag{2.18}$$

which is the sum over the isoscalar ($t = 0$) and isovector ($t = 1$) components. These are, in turn, written as

$$\chi_t(\boldsymbol{r}) = C_t^{\rho\rho}\rho_t^2 + C_t^{\rho\tau}\rho_t\tau_t + C_t^{JJ}\sum_{\mu\nu} J_{\mu\nu,t}J_{\mu\nu,t} + C_t^{\rho\Delta\rho}\rho_t\Delta\rho_t + C_t^{\rho\nabla J}\rho_t\nabla\cdot\boldsymbol{J}_t. \tag{2.19}$$

[explain what divJ is] The coefficients $C_t^{uu'}$ are real constants, except for traditional density-dependence

$$C_t^{\rho\rho} \equiv C_{t0}^{\rho\rho} + C_{t1}^{\rho\rho}\rho^{\gamma}. \tag{2.20}$$

[elaborate on origins of this density dependence]

Strictly speaking, the original Skyrme EDF [cite] was derived for Hartree-Fock theory, which does not include pairing effects. Historically, [note on pairing contributions to net binding energies], quite simple pairing terms have been used. If desired, one can rederive the Skyrme EDF in the pairing channel. The end result is that one simply replaces ph-densities with pp-densities everywhere in Eq. 2.19 except in the density-dependent coefficient $C_t^{\rho\rho}$. Modern EDFs use a simplified variant:

$$\mathcal{E}_{\rm pp} = \sum_q \frac{V_q}{2}\left[1 - \frac{1}{2}\left(\frac{\rho_0(\boldsymbol{r})}{\rho_c}\right)^{\beta}\right]\tilde{\rho}_q^2(\boldsymbol{r}), \tag{2.21}$$

see Ref. [1] and references therein. The isoscalar particle density is $\rho_0(\boldsymbol{r}) = \rho_p(\boldsymbol{r}) + \rho_n(\boldsymbol{r})$. The coefficients V_q, switching density ρ_c, and exponent β, are additional fit parameters. [comment on Fayans functional here]

[paragraph discussing various fits that are out there - at least unedf and skms]. now-dated review: Stone J and Reinhard P G 2007 Prog. Part. Nucl. Phys. 58 587

2.2.2 The Gogny EDF

The particle-hole part of the Gogny EDF, unlike the Skyrme EDF, is almost exclusively written in the literature as an effective two-body interaction, as

$$\hat{V}(\boldsymbol{r}_1, \boldsymbol{r}_2) = \sum_{i=1,2} e^{-(\boldsymbol{r}_1-\boldsymbol{r}_2)^2/\mu_i^2} \big(W_i + B_i \hat{P}_\sigma - H_i \hat{P}_\tau - M_i \hat{P}_\sigma \hat{P}_\tau\big) \tag{2.22a}$$

$$+ t_0\big(1 + x_0 \hat{P}_\sigma\big)\rho^\alpha\left(\frac{\boldsymbol{r}_1 + \boldsymbol{r}_2}{2}\right)\delta(\boldsymbol{r}_1 - \boldsymbol{r}_2) \tag{2.22b}$$

$$+ iW_{\mathrm{LS}}(\boldsymbol{\sigma}_1 + \boldsymbol{\sigma}_2) \cdot (\overleftarrow{\nabla}_1 - \overleftarrow{\nabla}_2) \times \delta(\boldsymbol{r}_1 - \boldsymbol{r}_2)(\overrightarrow{\nabla}_1 - \overrightarrow{\nabla}_2), \tag{2.22c}$$

see Refs. [7] [and others] The operators $\hat{P}_\sigma$, $\hat{P}_\tau$ are the spin and isospin exchange operators, respectively. The gradients operate to the left or right corresponding to the direction of the arrow above them. The terms μ_i, $W_i\, B_i\, H_i\, M_i\, t_0$, x_0, α, and W_{LS} are fit parameters.

One sees in this two-body interaction terms that are similar to the Skyrme effective interaction, which can be found in Ref. [11]. Indeed, expanding the first term, Eqn. (2.22a), about $\boldsymbol{r}_1 - \boldsymbol{r}_2 = 0$ precisely gives the contact terms in the Skyrme EDF. The approximate three-body force, Eqn. (2.22b), matches the density-dependent coefficient $C_t^{\rho\rho}[\rho]$ in the same approximation, and Eqn. (2.22c) corresponds to the spin-orbit term.

Various parameterizations exist [comment].

2.2.3 Other EDFs

Other EDFs include the Fayans [cite], BCPM [cite], others [cite]. Why are they interesting?

2.3 Constrained Calculations

The HFB equations can be solved with various constraints imposed, via the usual method of Lagrange multipliers. For any one-body operator, written in [form], one can simply do whatever. HFBTHO and others have clever ways of doing it; old literature mentions the various ways people have tried things before. Point out that expectation values of one-body operators have a generic form

2.3.1 Particle Number

The particle number operator is, in second-quantized form, $\hat{N} = \sum_k a_k^\dagger a_k$. Notice that the HFB wavefunction is not an eigenstate of this operator, i.e. the HFB wavefunction does not have definite particle number. This is problematic: we are describing finite nuclei, which have a definite number of protons and neutrons. Exact particle number restoration can be carried out in the framework of symmetry restoration, in which the HFB wavefunction is projected onto a desired eigenstate of $\hat{N}$, see refs [whatever]. Certainly, this has been carried out in a number of works, see [a bunch of refs].

In this work, we do not exactly restore particle number symmetry. Doing so is computationally expensive [elaborate] compared to a single HFB calculation. As such, no EDFs have been fit with restored PN [check!]. Since the EDF is phenomenological - it is not connected to the underlying nucleon-nucleon interaction in the way that, say, effective field theories are connected to QCD - it must be fit to some experimental data. The choice of many-body method should be considered as part of the fit [surely Witek talked about this somewhere], meaning that one should not fit an EDF at the HFB level, then use it with exact particle-number restoration.

Nevertheless, one can approximately restore particle number symmetry using the Lipkin-Nogami method. This also prevents pairing collapse, in which the effective pairing gap $\bar{\Delta}$ between quasiparticle levels vanishes, see Refs. whatever. In short, LN adds the following term to h_q:

The UNEDF1 functional mentioned above has also been fit using Lipkin-Nogami, blah blah blah. As such, we will distinguish the EDF used, denoting by $\text{UNEDF1}_{\text{HFB}}$ ($\text{UNEDF1}_{\text{LN}}$) the fit done at the HFB (LN) level.

Typically, one is reduced to constraining the average particle number, $\langle \text{HFB}|\hat{N}|\text{HFB}\rangle$, to the desired value. This is done for protons and neutrons separately. This has the effect of replacing the mean-field Hamiltonian h with

$$h_q \to h_q - \lambda_q, \tag{2.23}$$

with chemical potential λ_q. [elaborate on what this does/means]

2.3.2 The Nuclear Shape

As will be discussed later, our approach to nuclear fission requires understanding the energy cost required to deform a nucleus. This is done by carrying out HFB calculations with the nucleus constrained to a given shape. There are a number of different parameterizations, including [whatever]. A common choice is the multipole moments,

$$Q_{\mu\lambda} = asdf. \tag{2.24}$$

idk, probably a useful figure goes here, or else just reference Schunck's review for images

there

explicitly mention that our constraints here define the collective coordinates

2.3.3 Dynamical Pairing

I guess this is not a constraint, so much as an input

2.4 Further Discussion

DFT has been used and extended far beyond the scope of this thesis. Instead of attempting to describe the field in detail, we will instead briefly introduce many of the ways DFT has been used and extended, followed by references to relevant literature.

2.4.1 Time Dynamics

The world is, ultimately, a dynamical system. As such, time dynamics have long existed in the mean-field picture. Runge-Gross theorems [see [8] and refs within] prove similar results as the Hohenberg-Kohn theorems, but for time-dependent systems. For a discussion of TDDFT, and its adiabatic approximation, see Ref. [8] and references within [probably add some of those...maybe? maybe not worth it]. For the purposes of this work, all that is needed is the collective inertia tensor. Adiabatic TDDFT expands the usual TDDFT equation in a low-velocity approximation, and identifies a collective kinetic and potential energy. The former can be written as

$$\mathcal{K} = \frac{1}{2} \sum_{\alpha\beta} M_{\alpha\beta} \dot{q}_\alpha \dot{q}_\beta, \tag{2.25}$$

where the q_α are the collective coordinates defined above, the dot signifies their time derivative, and $M_{\alpha\beta}$ is the collective inertia tensor.

The exact calculation of M is fraught numerically [I think]. Instead, one commonly (and we, throughout this work) use the so-called perturbative cranking approximation ...

2.4.2 Beyond the Mean Field

DFT has been expanded on in many ways. To describe

2.4.3 Applications

Way too much to do

maybe discuss what else hfb has been used for, idk. probably adds to the discussion

- motivation for dft. essentially, schrodinger equation can't be solved exactly, but strong evidence for mean-field picture
- connection to quantum chemistry? brief mention of KS theorems?
- historical use of dft? for finite nuclei and nuclear matter?
- HF, BCS pairing, and HFB. since we work at HFB level, probably only need to discuss that
- write down summary of HFB equations: write $E[\rho, \tilde{\rho}]$, vary wrt ρ and $\tilde{\rho}$, end up with HFB matrix you diagonalize
- densities are now important; can just be summarized w/out too much detail. also discusses orbitals as necessary step
- write down Skyrme form of EDF; here, witek's form is sensible. mention time-odd terms; mention other forms that exist, but skyrme is most important for this work. emphasize pairing form of EDF?
- hfb wavefunction is not eigenstate of particle number. constrain average particle number; LN is also a thing, but not super important. also probably don't need to discuss symmetry restoration
- probably useful to enumerate some ways the edf has been calibrated, esp. unedf functionals
- constrain to multipole moments to carve out effective barrier - so mention how constraints are used
- probably helpful to mention the code(s) that're out there, esp. hfbtho

Chapter 3. Fission Observables

Actually, here can just leap right into the tunneling process, basically (no overview)

- Introduce types of fission: spontaneous and induced. Can start maybe with historical perspective, b/c I assume they first measured induced
- Describe observables for both: the classic timescale idea, and what pops out at different timescales. Most observables are the same for both: lifetimes, fragment yields (primary and cumulative), neutron multiplicities, etc
- Describe specific quantities that are different for induced vs spontaneous: cross section, mainly/only
- Primarily focus on SF. Dovetail into tunneling process vs outside-of-barrier processes
- Talk about tunneling first, even though it'll be longer discussion, b/c that's what happens first
- Discussion on post-tunneling process (Langevin, TDDFT, microcanonical)

Intro goes here

3.1 Overview

Schmidt2018 is a review

3.1.1 Spontaneous Fission

3.1.2 Induced Fission

3.2 The Tunneling Process

3.2.1 Previous Approaches

3.2.2 The Nudged Elastic Band

3.3 Primary Fragment Yields

3.3.1 Dynamical Approaches

TDDFT, Langevin - Abe1996 is good ref for langevin

3.3.2 Microcanonical Ensemble Approach

Chapter 4. Multimodal Fission

- Maybe just belongs as subset of fission observables discussion
- If not, is just a copy-paste job of multimodal paper

Chapter 5. Fission Emulators

- Start with computational challenge: model dependence from previous chapter
- Mention astrophysics applications as increased number of calculations required. Branch off into first problem: can we get one set of yields across the r process region, even w/out uncertainties?
- NN paper says: more or less, yea
- Reduced order models time!

Chapter 6. Conclusions/Outlook?

Bibliography

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