

Everything you wish you'd known when you  
STARTED your PhD

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Revised November 2017



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# Chapter 1

## Pairing in Nuclear Theory

There are several different ways to include pairing correlations in nuclear structure calculations, many of which are based on the BCS theory of superconductors. In it, nucleon pairs can be described as quasiparticles in a nuclear superfluid. Here I will describe three different approaches for describing nuclear structure which account for pairing, each with varying degrees of generality.

First I might ask you, though: why should we even do any specific considerations for pairing at all? Shouldn't the nuclear force contain the entire interaction? So then why do we invent things like HF-BCS or HFB where pairing is *separate* from the mean field interaction? Is pairing just an artificial construct? And my answer is that the question is somewhat misleading. Pairing isn't really related to the mean field, or even the nucleon-nucleon interaction. It's actually more a result of the Pauli exclusion principle and quantum orbitals and such. Pairs form when you have two nucleons in the same quantum state, except with opposite spin or isospin. Then they kind of just hang out with each other in the same places and do everything together because that's what pairs in the same quantum state do. So it kind of maybe amplifies the effect of the nucleon-nucleon interaction (or rather, the fact that other nucleons are found in separate orbitals might tend to damp it). This is true for mean field/DFT models; in shell model theories, there's no real need for this distinction (see [?]; is pairing even a meaningful concept in shell models?).

Just some terminology: **Pairing strength** refers to the coefficient of the *effective* pairing interaction. A large pairing strength means pairs are more likely to form. **Pairing gap** refers to the energy it takes to break a pair and promote one particle

to the next energy level. A large pairing gap keeps pairs together. Pairing strength and pairing gap are similar concepts and may be related in some cases; the difference is that one is a phenomenological construct used in effective theoretical descriptions whereas the other is a physically “measurable” quantity. **Pairing energy** refers to the extra binding energy associated with nucleonic pairs. It is (I believe) the energy contribution coming from the effective pairing interaction.

I should also mention that in the literature, there are two types of pairing that get mentioned: static and dynamic pairing correlations. So far as I can tell, **static pairing** refers to pairing at the level of HF+BCS or HFB. It might, for example, take the form of a density-dependent zero-range interaction such as this:

$$V(r) = V_0 \left( 1 - \left( \frac{\rho(r)}{\rho_0} \right)^\alpha \right)$$

I believe this is what you would use to create the  $\Delta$  in your HFB matrix, for instance.

**Dynamic pairing** refers to correlations that go beyond this approximation, and they are what cause so-called pairing fluctuations or pairing vibrations (if pairing correlations are strong enough and you start moving away from magic nuclei, the parameters defining the pairing gap will fluctuate or vibrate around their ground state value in the same way the surface shape might vibrate around its ground state shape). Essentially you can break down the energy like this:

$$E \rightarrow E_{HF} + E_{static}^{pair} + E_{dyn}^{pair} \equiv E_{HFB} + E_{dyn}^{pair}$$

I believe Lipkin Nogami is an example dynamic pairing recipe. In essence, you see pairs becoming more or less attached to their parent nucleus, and that in turn affects the dynamics. This is why Lipkin-Nogami keeps track of particle number: because the particle number of the nucleus is actually somewhat changing, as those pairs decide whether or not to stay attached (and I’m not sure whether I mean the pair would separate or if they would just be excited as a boson-like pair). By fixing the particle number as you do with Lipkin-Nogami, you essentially fix the gap strength, which determines how hard the nucleus has to work to keep that pair attached. Sometimes it’ll be worth it, and sometimes it won’t.

For more information on static vs dynamic pairing correlations, some possible starting points are this passage from 50 Years of Nuclear Pairing (figures 1.1 and

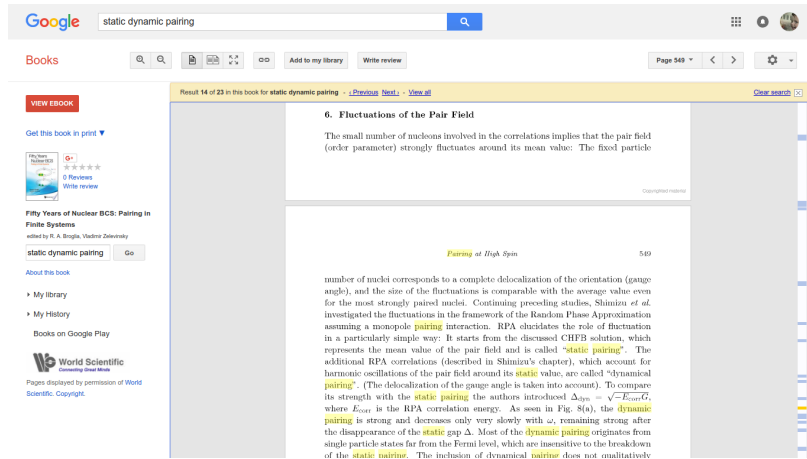


Figure 1.1: Part 1 of a helpful description of the difference between static and dynamic pairing.

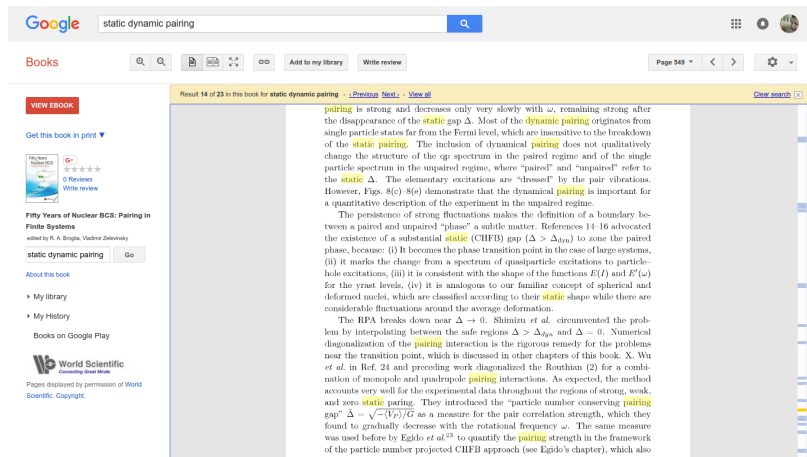


Figure 1.2: Part 2 of a helpful description of the difference between static and dynamic pairing.

1.2), along with this paper: [31]. To see how they play a role physically, see [30] and [18].

[Note: 14 November 2017] It turns out I'm not quite right about this. The "pure HFB/static pairing case" refers to the case described by  $H' = H - \lambda N$ . There are still (so far as I understand) dynamical pairing fluctuations. Then, once you add another term  $H'' = H' + \lambda_2 \Delta N^2$  you'll obtain even stronger pairing fluctuations

## BCS Theory and HF+BCS ([32, 3])

One way to include pairing correlations is to solve the Hartree-Fock equations and add BCS on top. This method is called HF+BCS and it does a fair job of describing nuclei near the valley of stability, but gets progressively worse the further from stability you get (see [3]).

Basically the idea is that you use HF to take you from a system with a whole bunch of interdependent particles, which each obey a one-body Hamiltonian piece AND a two-body Hamiltonian piece, to an alternate basis in which you basically only have a one-body Hamiltonian. Then, in that basis, you solve the BCS equations on top, so you're doing BCS on a basis that doesn't exactly describe the real interaction Hamiltonian but is close enough to the real thing.

Another way of saying it is that the HF equations give you single-particle wavefunctions, in the basis which most closely approximates/diagonalizes the [two-body] Hamiltonian. So it's sort of a fictitious basis, in that your Hamiltonian is not *really* diagonal, but it's as good as you're gonna get. That's what the variation does - you're varying the ground state energy according to the coefficients which give you the most ideal linear combination of starting basis functions (harmonic oscillator or whatever). But the main idea is this: that you pretend your two-body Hamiltonian is actually a one-body Hamiltonian, diagonalize it, and make the error in your approximation as small as possible.

For the next step, when you add in the BCS, you typically make (at least for even-even nuclei) the ground state ansatz  $|BCS\rangle = \prod_{k>0} (u_k + v_k a_k^\dagger a_k^\dagger) |0\rangle$ , which doesn't conserve particle number (in fact, it's a linear superposition of pairs starting from zero pairs all the way up to  $\frac{A}{2}$  pairs), but I guess it's close enough. Then you typically enforce particle number conservation some other way, perhaps by adding a Lagrange multiplier.

Next you take your pairing Hamiltonian, which I suppose would include your mean-field, now one-body Hamiltonian (which stands in for the two-body Hamiltonian you had before you performed Hartree-Fock), and you add in a new two-body potential, which this time represents the effect of pairing. Then you perform a Hartree-Fock-style calculation all over again, essentially just doing another Hartree-Fock calculation on top of your original one, except that this time you might probably



have an extra Lagrange multiplier constraint in your Hamiltonian. It doesn't change anything substantial but it's good to keep in mind. There are probably other ways of constraining particle number, too, like Lipkin-Nogami, but I'm not too sure how those work.

Some other things to keep in mind:

- You can still think of your system in terms of the HF-basis real particle wave-functions  $a_k^\dagger|0\rangle$ , with  $|BCS\rangle = \prod_{k>0}(u_k + v_k a_k^\dagger a_{\bar{k}}^\dagger)|0\rangle$ . Or, to simplify the math, you can invent a new "quasiparticle" such that  $|BCS\rangle = \prod_k \alpha_k^\dagger|0\rangle$ . This trick is called the Bogoliubov transformation and it looks like this:

$$\alpha_k^\dagger = u_k a_k^\dagger - v_k a_{\bar{k}} \quad (1.1)$$

$$\alpha_{\bar{k}}^\dagger = u_k a_{\bar{k}}^\dagger + v_k a_k \quad (1.2)$$

- A pairing gap  $\Delta = 0$  seems to mean there is no energy associated with pairing. All pairs are formed below the Fermi surface, because why on Earth wouldn't they? It's free! Whereas a nonzero pairing gap means there is some energy associated with forming a pair. So the probability of forming pairs is less than one below the Fermi surface, but there's also a possibility that pairs might form outside the Fermi surface. The pairing gap basically defines how far outside the Fermi surface you can go (see p 233 of [22], for ex., or p 13 of [4]).
- You could also do the BCS calculation using single-particle states derived from a phenomenological potential. You'd sacrifice some accuracy but gain some speed [3].

## Hartree-Fock-Bogoliubov (HFB) ([22, 4])

In HF theory, you find the eigenfunctions of the one-body Hamiltonian which most closely resembles the actual two-body Hamiltonian. The basic idea to HFB is that in HFB you do basically the same thing, except you can't ignore two-body interactions because of pairing. So I guess in a way you sort of find the eigenfunctions of the two-body Hamiltonian which most closely resembles the actual four-body Hamiltonian.

There's a little bit more subtlety than that, because the pairing correlations mean the particles are related somehow, but that's not a bad way to envision it, because one quasiparticle has a  $U$  term, which corresponds to adding a particle, and a  $V$  term, which does the opposite - so it's like creating a pair all at once (see equation 1.4)! In reality, each HFB quasiparticle is a sum of such terms, but you get the idea. In some sense, one quasiparticle  $\sim$  two real particles.

By way of comparison to HF+BCS, which is a two-step process, HFB just does both steps at once to give you a single set of quasiparticle wavefunctions, instead of one set of single-particle wavefunctions based on another set of wavefunctions. The approximation in the end is better, but it is more computationally intensive than HF+BCS.

Let's see how this calculation is to be done. Suppose our Hamiltonian is:

$$\hat{H} = \sum_{i,j} t_{ij} \hat{c}_i^\dagger \hat{c}_j + \frac{1}{4} \sum_{i,j,m,n} \bar{v}_{ijmn} \hat{c}_i^\dagger \hat{c}_j^\dagger \hat{c}_n \hat{c}_m \quad (1.3)$$

As mentioned before, let us make the following Bogoliubov transformation to make the math simpler:

$$\begin{pmatrix} \hat{\beta} \\ \hat{\beta}^\dagger \end{pmatrix} = \begin{pmatrix} U^\dagger & V^\dagger \\ V^\dagger & U^\dagger \end{pmatrix} \begin{pmatrix} \hat{c} \\ \hat{c}^\dagger \end{pmatrix} \quad (1.4)$$

Now the Hamiltonian looks like this:

$$\begin{aligned} \hat{H} &= \hat{H}_0 + \sum_{i,j} \hat{H}_{i,j} \beta_i^\dagger \beta_j + \sum_{i < j} (\hat{H}_{i,j} \beta_i^\dagger \beta_j^\dagger + h.c.) + \hat{H}_{int} \\ &= \hat{H}_0 + \hat{H}_{11} + \hat{H}_{20} + \hat{H}_{40} + \hat{H}_{31} + \hat{H}_{22} \end{aligned} \quad (1.5)$$

where  $h.c.$  is the hermitian conjugate of the previous term and the term  $\hat{H}_{nm}$  contains all terms with  $n$  quasiparticle creation operators and  $m$  annihilation operators. We'll lump the terms with 4 creation/annihilation operators into a single term  $\hat{H}_{int}$ , which we'll assume is small and thus ignore (sort of like the term  $V(r) - \sum_{i,j} V(r_i, r_j)$  from regular Hartree-Fock theory). Let us constrain the average particle number by adding in a Lagrange multiplier term  $\lambda N$ . Then we vary the total energy with respect to  $U$  and  $V$  (which are matrices):

$$\delta E' = \langle \Phi_0 | \hat{H} - \lambda \hat{N} | \Phi_0 \rangle \quad (1.6)$$

After that, it's really just algebra. The variation leaves some ambiguity still in the choice of  $U$  and  $V$ , so we will choose them to make  $\hat{H}_{20} = 0$  and  $\hat{H}_{11}$  diagonal. Additionally, the solution will look nicer if we introduce the following two densities, the traditional single-particle density from Hartree-Fock  $\rho$  and a pairing tensor called  $\kappa$ :

$$\rho_{ij} = \langle \Phi_0 | \hat{c}_j^\dagger \hat{c}_i | \Phi_0 \rangle = (VV^T)_{ij} \quad (1.7)$$

$$\kappa_{ij} = \langle \Phi_0 | \hat{c}_j \hat{c}_i | \Phi_0 \rangle = (VU^T)_{ij} \quad (1.8)$$

I'd just like to mention something here that Nicolas also mentions in his notes: that you can think of the single-particle density as sort of an overlap between one state with  $n$  particles ( $\langle \Phi_0 | \hat{c}_j^\dagger \hat{c}_i$ ) and another state which *also* has  $n$  particles ( $|\Phi_0\rangle$ ), while the pairing tensor acts as a sort of probe of the interaction between states with  $n$  particles ( $|\Phi_0\rangle$ ) and a state with  $n + 2$  particles ( $\langle \Phi_0 | \hat{c}_j \hat{c}_i$ ).

We can make things look *even nicer* if we introduce the following notation representing the mean field  $\Gamma$  and the pairing field  $\Delta$ :

$$\Gamma_{kl} = \sum_{i,j} \bar{v}_{kjl} \rho_{ij} \quad (1.9)$$

$$\Delta_{kl} = \frac{1}{2} \sum_{i,j} \bar{v}_{kl} \kappa_{ij} \quad (1.10)$$

After we make all these substitutions, the Hamiltonian looks like:

$$\hat{H} - \lambda \hat{N} = \sum_{i,j} \left( \left( t_{ij} + \frac{1}{2} \Gamma_{ij} - \lambda \right) \rho_{ji} + \frac{1}{2} \Delta_{ij} \kappa_{ji}^* \right) + \sum_i E_i \hat{\beta}_i^\dagger \hat{\beta}_i + \hat{H}_{int} \quad (1.11)$$

where  $\hat{H}_{int}$  contains all the terms with four creation/annihilation operators and  $\sum_i E_i \hat{\beta}_i^\dagger \hat{\beta}_i$  is the diagonal form of  $\hat{H}_{11}$ .

Finally, putting everything back in terms of the real particle creation and annihilation operators  $c_i^\dagger$  and  $c_i$  (and then dropping those in favor of their coefficients),

we get the Hartree-Fock-Bogoliubov equations in their most familiar form (setting  $h = \epsilon + \Gamma$ ):

$$\begin{pmatrix} h - \lambda & \Delta \\ -\Delta^* & -(h - \lambda)^* \end{pmatrix} \begin{pmatrix} \hat{U}_k \\ \hat{V}_k \end{pmatrix} = E_k \begin{pmatrix} \hat{U}_k \\ \hat{V}_k \end{pmatrix} \quad (1.12)$$

The case of rotating nuclei is interesting because experimental moments of inertia of deformed nuclei are found to be 2-3 times larger than what is calculated when pairing is ignored. Suhonen interprets this to mean that actual rotations involve the superfluid valence pairs rotating around an inert core. You can treat this by adding another constraint to  $\hat{H} - \lambda\hat{N} - \omega J_x$ . This is the idea behind what is called the cranking model, which describes systems in a rotating frame. It violates time-reversal just like how you've already eliminated particle number conservation. And you can add other constraints  $\hat{H} - \lambda\hat{N} - \lambda_i\hat{Q}_i$  for any number of other things, like shape deformations. We use these in fission a lot.

## Just a note...

...and I'm not sure where exactly to put this, but here goes: I like the idea of recasting nuclear structure, and especially applications with heavy nuclei such as fission, in terms of a DFT framework, because in principle a DFT framework is (or can be) exact as a way of taking into account all the quantum properties of the underlying nuclear degrees of freedom. And if you're clever about it, you can use ab initio approaches to inform or develop new and useful EDFs. But I don't know what would be the best way to do that. If you just fit a Skyrme functional to some quantities calculated by an ab initio method, you really aren't doing anything better than just fitting it to experimental quantities - in fact, the experimental quantities should in principle be better! So there's a non-trivial issue to solve. It seems like something that should be doable - use an ab initio method to derive a new type of EDF with perhaps a new and better parameterization, but right now that bridge feels like a missing link. There might be some hints, though, in the references found in section 2.3 of [28]

## Chapter 2

# Time-dependent Hartree-Fock and the inertia tensor

Originally this development is based on [12], and a retelling in notes by Nicolas which I have on paper but not digitally.

Some of this (specifically that relating to the inertia tensor and the cranking approximation) is mentioned in [5]

The HFB matrix looks different depending on your basis (obviously...). In the single-particle basis, it has the form

$$\mathcal{H} = \begin{pmatrix} h & \Delta \\ -\Delta^* & -h^* \end{pmatrix} \quad (2.1)$$

with an associated density

$$\mathcal{R} = \begin{pmatrix} \rho & \kappa \\ -\kappa^* & 1 - \rho^* \end{pmatrix} \quad (2.2)$$

Or something like that. I might have the signs and stars wrong.

In the quasiparticle basis, on the other hand, these matrices look like this:

$$\mathcal{H} = \begin{pmatrix} E & 0 \\ 0 & -E \end{pmatrix}, \mathcal{R} = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} \quad (2.3)$$

At finite temperatures  $T > 0$ , the density is slightly modified:

$$\mathcal{R} = \begin{pmatrix} f & 0 \\ 0 & 1 - f \end{pmatrix} \quad (2.4)$$

What is done in ATDHFB (and, so far as I can tell, also in QRPA) is to expand your density  $\mathcal{R}$  around some  $\mathcal{R}_0$ , which in QRPA corresponds to the HFB ground state density (I think) and in ATDHFB *can* be the HFB ground state density (in practice, I think that is indeed what's most often done). The expansion parameter  $\chi(t)$  works out to be, in some sense, a canonical coordinate or momentum or something like unto it. For small perturbations around the minimum, the system looks like a harmonic oscillator in time, described by the ATDHFB equations  $i\dot{\mathcal{R}} = [\mathcal{H}, \mathcal{R}]$ . In ATDHFB, you find that the most common perturbations are collective coordinate changes (corresponding to shape deformations). Writing your derivatives in terms of these collective variables

$$\frac{d\mathcal{R}}{dt} = \frac{d\mathcal{R}}{dq} \frac{dq}{dt} \quad (2.5)$$

and then writing everything in terms of  $\chi(t)$  and  $\dot{\chi}(t)$ , you find an expression for the energy which looks like a kinetic energy, with  $\dot{q}$ 's or  $\dot{\chi}$ 's as your "velocity."

Begin by expanding  $\mathcal{R} \approx \mathcal{R}_0 + \mathcal{R}_1$  and, correspondingly,  $\mathcal{H} \approx \mathcal{H}_0 + \mathcal{H}_1$ .  $\mathcal{R}_0$  and  $\mathcal{H}_0$  are both diagonal in the quasiparticle basis, so it makes sense to start from there. Expand your commutator  $i\dot{\mathcal{R}} = [\mathcal{H}, \mathcal{R}]$  in terms of these guys where possible, and a lot of this stuff will turn out to be pretty trivial. The difficult part will be expressing  $\mathcal{H}_1$  in the quasiparticle basis. For that, you'll probably need to start with  $\mathcal{R}$  and  $\mathcal{H}$  in the single-particle basis

$$\mathcal{R} = \begin{pmatrix} \rho & \kappa \\ -\kappa^* & 1 - \rho^* \end{pmatrix} \approx \begin{pmatrix} \rho_0 & \kappa_0 \\ -\kappa_0^* & 1 - \rho_0^* \end{pmatrix} + \begin{pmatrix} \rho_1 & \kappa_1 \\ -\kappa_1^* & -\rho_1^* \end{pmatrix} \quad (2.6)$$

Then you'll construct  $\mathcal{H}$  in this basis by explicitly evaluating  $h_{ij} = t_{ij} + \sum_{mn} \bar{v}_{imjn} \rho_{nm}$  and  $\Delta_{ij} = \frac{1}{2} \sum_{mn} \bar{v}_{ijmn} \kappa_{mn}$  (double-check the indices and expressions before use, of course!). You can transform this into the quasiparticle basis, or the other part into the single particle basis (or in reality, I think you'll have to do a bit of both), and that'll give you the full expression. However, in the cranking approximation, we actually apparently ignore this whole second term because we assume that small changes in the density will not affect the mean field ( $\mathcal{R} \approx \mathcal{R}_0 \Rightarrow \mathcal{H}_1 \approx 0$ )

To close out this chapter, a good soul-searching question you should ask yourself someday (just to make sure you understand what's going on) is, if you take away the ATDHFB or GCM or and other model-dependence, what is still left? What is the essence of the inertia tensor, and what do you risk leaving behind in each of these models? Because the inertia tensor exists even in older models, too. Clearly, there's something that people associate with a collective inertia that dates back many years.





## Chapter 3

# RPA vs ATDHF and QRPA vs ATDHFB

I suspect the "Random Phase" in RPA refers to the  $\chi$  which pops up when we rewrite the density  $\rho$  about the HF/HFB ground state density  $\rho_0$  in the following way:

$$\rho = e^{i\chi} \rho_0 e^{-i\chi} \quad (3.1)$$

The "Approximation" part of RPA is when we expand  $\rho$  for small perturbations about the ground state, truncating the series at (typically) first- or second-order in  $\chi$ .

In static RPA, once we've expanded the density and the energy out to second-order in  $\chi$ , you can rewrite the second-order energy term as a vector-matrix-vector multiplication:

$$E^{(2)} = \frac{1}{2} (\chi^\dagger, -\chi^T) \begin{pmatrix} A & B \\ B^* & A^* \end{pmatrix} \begin{pmatrix} \chi \\ -\chi^* \end{pmatrix} \quad (3.2)$$

This matrix is what is called the RPA matrix (or sometimes the stability matrix, since  $|E^{(2)}| > 0$  corresponds to  $\rho_0$  being a minimum, I think).

This matrix actually pops up again when you start from the TDHF equations  $i\hbar \frac{\partial \rho}{\partial t} = [h, \rho]$ . Expand the density around its ground state in terms of some parameter  $\chi$  again, except this time,  $\chi$  is time-dependent. If you work in the HF basis where the density and the energy are both diagonal, and keeping terms to first order this time, you eventually arrive at

$$i\hbar(n_j - n_i)\frac{\partial}{\partial t} \begin{pmatrix} \chi_{ij} \\ \chi_{ij}^* \end{pmatrix} = \begin{pmatrix} A_{ij\mu\nu} & B_{ij\mu\nu} \\ B_{ij\mu\nu}^* & A_{ij\mu\nu}^* \end{pmatrix} \begin{pmatrix} \chi_{\mu\nu} \\ -\chi_{\mu\nu}^* \end{pmatrix} \quad (3.3)$$

So apparently this matrix is significant somehow.

Something worth mentioning is that, at least according to [6], RPA is essentially the small-amplitude limit of ATDHFB. I haven't gone into any more detail than that for right now, but it seems like something that bears repeating.

Another thing that I have written down that I know will be worth mentioning is that RPA correlations tend to increase the effective mass. I'm not sure where I read that, but I must have read it somewhere.

An additional thing, which isn't particularly relevant here but which I have written on the same piece of scratch paper, is that having many nucleons tends to destroy shell effects.

## ATDHFB vs GCM

I'll only give this a small section for now until I study GCM in more depth someday, but another recipe one can use to estimate the inertia tensor (which we'll see in the next chapter) is the Generator Coordinate Method. I'm not too familiar with it, but I know that it apparently neglects/lacks some time-odd terms which cause it to underestimate the mass of a nucleus undergoing translation. Furthermore, the GCM inertia tends to be smaller in magnitude than the ATDHFB inertia in general. Consequently, many people think that GCM is probably inferior to ATDHFB as a way of computing collective inertias. But since the collective inertia is not an observable quantity, there's no way to say for sure, so GCM is still oftentimes computed (I'm guessing it must be pretty cheap to compute perturbatively so why not?) and it's something you may as well use just to compare, you know?

# Chapter 4

## Temperature-dependent ATDHFB

A lot of these ideas I'm getting from [25] as well as Nicolas' own temperature-dependent HFB notes.

### 4.1 A brief overview of the theory

As in any statistical theory, one first must determine which sort of ensemble properly describes the system. Nuclei have (in principle) conserved number of particles; however in HFB theory, that's somewhat flexible since the BCS transformation explicitly breaks particle number symmetry. In principle we should perhaps use a microcanonical ensemble to describe a nucleus as a closed, isolated system, but that turns out to be challenging to solve because it requires a full knowledge of the eigenspectrum of the nucleus. Using that quirk of HFB theory, we wiggle our way out of this hairiness<sup>1</sup> to instead describe our system using the grand canonical ensemble, and this turns out to be tractable.

Moving forward by minimizing the grand potential  $\Omega$  gives us for the density:

$$\hat{D} = \frac{1}{Z} e^{-\beta(\hat{H} - \mu\hat{N})}$$

with associated partition function

$$Z = \text{Tr} \left[ e^{-\beta(\hat{H} - \mu\hat{N})} \right]$$

---

<sup>1</sup>You can wave your hands here and say that finite temperatures let you break superfluid pairs, and so the number of “quasiparticles” (which you could argue might have referred to pairs before but now might also include individual particles) can change.

Getting specifically to our particular choice of mean-field Hamiltonian, we substitute in some one-body operator for the exponent:

$$\hat{D}_{HF} = \frac{1}{Z} e^{-\beta \hat{K}}, Z = \text{Tr} \left[ e^{-\beta \hat{K}} \right]$$

where in the plain ol' Hartree Fock case,  $\hat{K} = \sum_{ij} K_{ij} c_i^\dagger c_j$  (in the HFB case,  $\hat{K}$  is a sum of all different one-body operator types, but it's the same basic idea).

Defining the HF density matrix  $\rho_{ij} = \text{Tr} \left[ \hat{D}_{HF} c_j^\dagger c_i \right]$ , we can show the following useful correspondence relations:

$$\rho = \frac{1}{1 + e^{\beta \hat{K}}} \\ \text{Tr} \left[ \hat{D}_{HF} \hat{A} \right] = \text{tr} \left[ \rho \hat{A} \right] = \sum_{ij} \rho_{ij} \hat{A}_{ij}$$

where  $\hat{A}$  is some operator in the single-particle basis. Similar things happen for the HFB case. At the end of the day in HFB, things work out to be pretty similar to the way they were before, except the density in the quasiparticle basis is replaced by

$$\mathcal{R} = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} \rightarrow \begin{pmatrix} f & 0 \\ 0 & 1 - f \end{pmatrix}$$

with the Fermi factor  $f$  given by  $f_\mu = \frac{1}{1 + e^{\beta E_\mu}}$ . Obviously there's a lot more richness to it than that, but this helps to at least see the basic skeleton of what changes at finite temperature.

## 4.2 Temperature-Dependent ATDHFB

Let us quickly review the essence of Time-Dependent Hartree-Fock-Bogoliubov (TDHFB). The fundamental assumption of TDHFB is that a system which is a Slater determinant at time  $t = 0$  and which is then allowed to evolve in time will remain a Slater determinant at all times  $t$ . This assumption allows us to write the TDHFB equation:

$$i\hbar \dot{\mathcal{R}} = [\mathcal{H}, \mathcal{R}]$$

where in the single-particle basis

$$\tilde{\mathcal{H}} = \begin{pmatrix} h - \lambda & \Delta \\ -\Delta^* & -h^* + \lambda \end{pmatrix}, \quad \tilde{\mathcal{R}} = \begin{pmatrix} \rho & \kappa \\ -\kappa^* & 1 - \rho^* \end{pmatrix}$$

The *additional* assumption that collective motion is slow compared to single particle motion of the system is called the *adiabtic approximation*, and the consequent model is called Adiabatic Time-Dependent Hartree-Fock-Bogoliubov (ATDHFB). Historically, the reason for this assumption comes from microscopic-macroscopic models of nuclear fission, where the dynamics of the system are described by a few collective shape variables and their derivatives (you might think of them semiclassically as coordinates and velocities). The adiabatic approximation is implicit in this assumption. ATDHFB provides the bridge for bringing this useful framework into a self-consistent, fully-microscopic picture.

Once the system is described in terms of collective coordinates and velocities, the energy can be expressed as the sum of a “potential” term (which depends on the coordinates) and a “kinetic” term (which depends on the velocities). Our goal is to understand the kinetic part of the energy, which in some sense describes the dynamics of, for example, a fissioning nucleus, in terms of the first few multipole moments of the nucleus. A key component of this will be the inertia tensor  $\mathcal{M}$ , which plays the role of the “mass”:  $E_{kin} \sim \frac{1}{2}\mathcal{M}\dot{q}^2$

### 4.2.1 Review of ATDHFB

With the adiabatic assumption in place, we can write the density as an expansion around some time-even zeroth-order density:

$$\begin{aligned} \mathcal{R}(t) &= e^{i\chi(t)}\mathcal{R}_0(t)e^{-i\chi(t)} \\ &= \mathcal{R}_0 + \mathcal{R}_1 + \mathcal{R}_2 + \dots \end{aligned}$$

where  $\chi$  is assumed to be “small” (which is explained more rigorously in [6]) and

$$\mathcal{R}_1 = i[\chi, \mathcal{R}_0] \tag{4.1}$$

$$\mathcal{R}_2 = \frac{1}{2}[[\chi, \mathcal{R}_0], \chi] \tag{4.2}$$

The HFB matrix, being a function of  $\mathcal{R}$ , is likewise expanded:

$$\mathcal{H} = \mathcal{H}_0 + \mathcal{H}_1 + \mathcal{H}_2 + \dots$$

and together  $\mathcal{R}$  and  $\mathcal{H}$  are plugged into the TDHFB equation. Gathering terms in powers of  $\chi$ :

$$i\hbar\dot{\mathcal{R}}_0 = [\mathcal{H}_0, \mathcal{R}_1] + [\mathcal{H}_1, \mathcal{R}_0] \quad (4.3)$$

$$i\hbar\dot{\mathcal{R}}_1 = [\mathcal{H}_0, \mathcal{R}_0] + [\mathcal{H}_0, \mathcal{R}_2] + [\mathcal{H}_1, \mathcal{R}_1] + [\mathcal{H}_2, \mathcal{R}_0] \quad (4.4)$$

These two equations are the ATDHFB equations. They can be solved self-consistently to find both  $\chi$  and  $\mathcal{R}_0$ ; however, this is rarely done in practice. More commonly what is done is to exploit the fact that solutions to the ATDHFB equations are (by design) *close* to true HFB solutions. We then take HFB solutions and compute their time derivatives by the first ATDHFB equation to get ATDHFB-like behavior without going through the full trouble of ATDHFB.

One nice feature of using true HFB solutions instead of ATDHFB solutions is that the matrix  $\mathcal{H}_0$  is diagonal in the HFB basis.

Finally, the total energy of the system is found to be

$$E(\mathcal{R}) = E_{HFB} + \frac{1}{2}\text{Tr}(\mathcal{H}_0\mathcal{R}_1) + \frac{1}{2}\text{Tr}(\mathcal{H}_0\mathcal{R}_2) + \frac{1}{4}\text{Tr}(\mathcal{H}_1\mathcal{R}_1)$$

The “kinetic energy” of the system is given by the latter two terms, which (as I’ll show explicitly in a moment), are both second order in  $\chi$ .

### 4.2.2 Relation between $\chi$ and $\dot{\mathcal{R}}$

Eventually we’ll want to express the energy in terms of the multipole moments  $q$  and their derivatives, but for now we will content ourselves with expressing the energy in terms of  $\mathcal{R}$  and  $\dot{\mathcal{R}}$ . From the first ATDHFB equation:

$$i\hbar\dot{\mathcal{R}}_0 = [\mathcal{H}_0, \mathcal{R}_1] + [\mathcal{H}_1, \mathcal{R}_0]$$

Working in the HFB quasiparticle basis, we have (at finite temperatures)

$$\mathcal{H}_0 = \begin{pmatrix} E & 0 \\ 0 & -E \end{pmatrix}, \quad \mathcal{R}_0 = \begin{pmatrix} f & 0 \\ 0 & 1-f \end{pmatrix}$$

Note that the block matrices  $E$  and  $f$  are both diagonal. In this same basis, we can also divide the perturbation matrix  $\chi$  and the first-order energy  $\mathcal{H}_1$  in the same block matrix form:

$$\chi = \begin{pmatrix} \chi^{11} & \chi^{12} \\ \chi^{21} & \chi^{22} \end{pmatrix}, \quad \mathcal{H}_1 = \begin{pmatrix} \mathcal{H}_1^{11} & \mathcal{H}_1^{12} \\ \mathcal{H}_1^{21} & \mathcal{H}_1^{22} \end{pmatrix}$$

Ultimately, by using the equations 4.1, we arrive at the result:

$$\begin{aligned} \hbar \dot{\mathcal{R}}_{(0),ab}^{11} &= (E_a - E_b)(f_b - f_a)\chi_{ab}^{11} + (f_b - f_a)\mathcal{H}_{(1),ab}^{11} \\ \hbar \dot{\mathcal{R}}_{(0),ab}^{12} &= (E_a + E_b)(1 - (f_a + f_b))\chi_{ab}^{12} + (1 - (f_a + f_b))\mathcal{H}_{(1),ab}^{12} \\ \hbar \dot{\mathcal{R}}_{(0),ab}^{21} &= (E_a + E_b)(1 - (f_a + f_b))\chi_{ab}^{21} - (1 - (f_a + f_b))\mathcal{H}_{(1),ab}^{21} \\ \hbar \dot{\mathcal{R}}_{(0),ab}^{22} &= (E_a - E_b)(f_b - f_a)\chi_{ab}^{22} - (f_b - f_a)\mathcal{H}_{(1),ab}^{22} \end{aligned} \quad (4.5)$$

It is common (the so-called “cranking approximation”) to assume that changes in the density have approximately no effect on the mean field, in which case these relations reduce to

$$\begin{aligned} \hbar \dot{\mathcal{R}}_{(0),ab}^{11} &= (E_a - E_b)(f_b - f_a)\chi_{ab}^{11} \\ \hbar \dot{\mathcal{R}}_{(0),ab}^{12} &= (E_a + E_b)(1 - (f_a + f_b))\chi_{ab}^{12} \\ \hbar \dot{\mathcal{R}}_{(0),ab}^{21} &= (E_a + E_b)(1 - (f_a + f_b))\chi_{ab}^{21} \\ \hbar \dot{\mathcal{R}}_{(0),ab}^{22} &= (E_a - E_b)(f_b - f_a)\chi_{ab}^{22} \end{aligned} \quad (4.6)$$

*Sanity Check:* In the  $T = f = 0$  case, the <sup>11</sup> and <sup>22</sup> terms vanish completely and we are left with the familiar [zero-temperature] ATDHFB equations:

$$\begin{aligned} \hbar \dot{\mathcal{R}}_{(0),ab}^{12} &= (E_a + E_b)\chi_{ab}^{12} + \mathcal{H}_{(1),ab}^{12} \\ \hbar \dot{\mathcal{R}}_{(0),ab}^{21} &= (E_a + E_b)\chi_{ab}^{21} - \mathcal{H}_{(1),ab}^{21} \end{aligned}$$

Another thing we must be careful of is the case of degenerate states. In such an event,  $E_a = E_b$  and  $f_a = f_b$ , leading again to  $\dot{\mathcal{R}}_{(0),ab}^{11} = \dot{\mathcal{R}}_{(0),ab}^{22} = 0$  (but I emphasize that this is only for this particular pair of states  $|a\rangle$  and  $|b\rangle$ ).

A third, rather pedantic case to be aware of is the example of a two-state system. In that case,  $f_a + f_b = 1$  and then the opposite happens; namely,  $\dot{\mathcal{R}}_{(0),ab}^{12} = \dot{\mathcal{R}}_{(0),ab}^{21} = 0$  while  $\dot{\mathcal{R}}_{(0),ab}^{11} \neq 0, \dot{\mathcal{R}}_{(0),ab}^{22} \neq 0$

### 4.2.3 Kinetic Energy at Finite Temperature

As mentioned previously, the expression for the “kinetic” energy of the system is given by:

$$E_{kin}(\mathcal{R}) = \frac{1}{2}\text{Tr}(\mathcal{H}_0\mathcal{R}_2) + \frac{1}{4}\text{Tr}(\mathcal{H}_1\mathcal{R}_1)$$

**Term proportional to  $\mathcal{R}_2$**

It can be shown that

$$\text{Tr}(\mathcal{H}_0\mathcal{R}_2) = \frac{1}{2}\text{Tr}([\chi, \mathcal{H}_0][\chi, \mathcal{R}_0])$$

which leads to

$$[\chi, \mathcal{H}_0] = \begin{pmatrix} [\chi^{11}, E] & -\{\chi^{12}, E\} \\ \{\chi^{21}, E\} & -[\chi^{22}, E] \end{pmatrix}, \quad [\chi, \mathcal{R}_0] = \begin{pmatrix} [\chi^{11}, f] & \chi^{12} - \{\chi^{12}, f\} \\ -\chi^{21} + \{\chi^{21}, f\} & -[\chi^{22}, f] \end{pmatrix}$$

$$\begin{aligned} \text{Tr}(\mathcal{H}_0\mathcal{R}_2) &= \frac{1}{2}\text{Tr}([\chi^{11}, E][\chi^{11}, f] + \{\chi^{12}, E\}(\chi^{21} - \{\chi^{21}, f\}) \\ &\quad + \{\chi^{21}, E\}(\chi^{12} - \{\chi^{12}, f\}) + [\chi^{22}, E][\chi^{22}, f]) \end{aligned} \quad (4.7)$$

Since  $E$  and  $f$  are diagonal, we can simplify expressions involving commutators and anticommutators. If  $A$  is an arbitrary matrix and  $D$  is diagonal, then

$$\begin{aligned} [A, D]_{\mu\nu} &= (D_\nu - D_\mu)A_{\mu\nu} \\ \{A, D\}_{\mu\nu} &= (D_\mu + D_\nu)A_{\mu\nu} \\ A_{\mu\nu} - \{A, D\}_{\mu\nu} &= (1 - D_\mu - D_\nu)A_{\mu\nu} \end{aligned}$$

Then this energy term becomes



$$\begin{aligned} \frac{1}{2} \text{Tr}(\mathcal{H}_0 \mathcal{R}_2) = \frac{1}{4} [ & (E_b - E_a)(f_a - f_b) \chi_{ab}^{11} \chi_{ba}^{11} + (E_a + E_b)(1 - f_a - f_b) \chi_{ab}^{12} \chi_{ba}^{21} \\ & + (E_a + E_b)(1 - f_a - f_b) \chi_{ab}^{21} \chi_{ba}^{12} + (E_b - E_a)(f_a - f_b) \chi_{ab}^{22} \chi_{ba}^{22} ] \end{aligned}$$

If you wanted to get *really* crazy (and we'll see in a bit why this might actually be okay), you could even throw in some extra delta functions to get this:

$$\begin{aligned} \frac{1}{2} \text{Tr}(\mathcal{H}_0 \mathcal{R}_2) = \frac{1}{4} [ & (E_b - E_a)(f_a - f_b) \delta_{a\alpha} \delta_{b\beta} \chi_{\alpha\beta}^{11} \chi_{ba}^{11} + (E_a + E_b)(1 - f_a - f_b) \delta_{a\alpha} \delta_{b\beta} \chi_{\alpha\beta}^{12} \chi_{ba}^{21} \\ & + (E_a + E_b)(1 - f_a - f_b) \delta_{a\alpha} \delta_{b\beta} \chi_{\alpha\beta}^{21} \chi_{ba}^{12} + (E_b - E_a)(f_a - f_b) \delta_{a\alpha} \delta_{b\beta} \chi_{\alpha\beta}^{22} \chi_{ba}^{22} ] \end{aligned}$$

Note that this now has the general form

$$\frac{1}{2} \text{Tr}(\mathcal{H}_0 \mathcal{R}_2) = \bar{\mathcal{M}}'_{\alpha\beta ab}{}^{11,11} \chi_{\alpha\beta}^{11} \chi_{ba}^{11} + \bar{\mathcal{M}}'_{\alpha\beta ab}{}^{12,21} \chi_{\alpha\beta}^{12} \chi_{ba}^{21} + \bar{\mathcal{M}}'_{\alpha\beta ab}{}^{21,12} \chi_{\alpha\beta}^{21} \chi_{ba}^{12} + \bar{\mathcal{M}}'_{\alpha\beta ab}{}^{22,22} \chi_{\alpha\beta}^{22} \chi_{ba}^{22} \quad (4.8)$$

where everything that isn't a  $\chi$  has just been kind of absorbed into a single coefficient.

Let's pause here for just a second and think about what we just did. Remember that our goal all along has been to treat this piece of the energy as sort of a "kinetic energy term" describing motion in a space of collective shape deformation coordinates. Then just now we found that, sure enough, we can factor this particular chunk into something that looks *kind of* like  $\frac{1}{2}mv^2$ . And we already know from 4.6 that  $\chi$  is related to  $\dot{\mathcal{R}}_0$ . Eventually we'll try to relate  $\dot{\mathcal{R}}_0$  to the collective shape coordinates  $\dot{q}$ , but first let's see if we can't get the other piece of the kinetic energy into the same form.

### Term proportional to $\mathcal{R}_1$

Recall that  $\mathcal{R}_1 = i[\chi, \mathcal{R}_0]$ ; then we can almost copy from equation 4.7 of the previous section:

$$\begin{aligned}
\frac{1}{4}\text{Tr}(\mathcal{H}_1\mathcal{R}_1) &= \frac{i}{4}\text{Tr}(\mathcal{H}_1^{11}[\chi^{11}, f] - \mathcal{H}_1^{12}(\chi^{21} - \{\chi^{21}, f\}) \\
&\quad + \mathcal{H}_1^{21}(\chi^{12} - \{\chi^{12}, f\}) - \mathcal{H}_1^{22}[\chi^{22}, f]) \\
&= \frac{i}{4}(\mathcal{H}_{(1),ab}^{11}(f_a - f_b)\chi_{ba}^{11} - \mathcal{H}_{(1),ab}^{12}(1 - f_a - f_b)\chi_{ba}^{21} \\
&\quad + \mathcal{H}_{(1),ab}^{21}(1 - f_a - f_b)\chi_{ba}^{12} - \mathcal{H}_{(1),ab}^{22}(f_a - f_b)\chi_{ba}^{22}) \quad (4.9)
\end{aligned}$$

But what are those  $\mathcal{H}^1$  terms? Since the interaction is known in the single-particle basis, we'll have to transform our density into the single-particle basis  $\mathcal{R}_1 \rightarrow \tilde{\mathcal{R}}_1$ , evaluate  $\tilde{\mathcal{H}}_1$  (which depends on  $\tilde{\mathcal{R}}_1$ ) in this basis, and then transform the result back into the quasiparticle basis  $\tilde{\mathcal{H}}_1 \rightarrow \mathcal{H}_1$

$$\tilde{\mathcal{R}}_1 = \begin{pmatrix} \rho_1 & \kappa_1 \\ -\kappa_1^* & -\rho_1^* \end{pmatrix} = i \begin{pmatrix} U & V^* \\ V & U^* \end{pmatrix} \begin{pmatrix} [\chi^{11}, f] & \chi^{12} - \{\chi^{12}, f\} \\ -\chi^{21} + \{\chi^{21}, f\} & -[\chi^{22}, f] \end{pmatrix} \begin{pmatrix} U^\dagger & V^\dagger \\ V^T & U^T \end{pmatrix}$$

$$\begin{aligned}
\Rightarrow \quad \rho_1 &= i(U[\chi^{11}, f]U^\dagger + U(\chi^{12} - \{\chi^{12}, f\})V^T - V^*(\chi^{21} - \{\chi^{21}, f\})U^\dagger - V^*[\chi^{22}, f]V^T) \\
\kappa_1 &= i(U[\chi^{11}, f]V^\dagger + U(\chi^{12} - \{\chi^{12}, f\})U^T - V^*(\chi^{21} - \{\chi^{21}, f\})V^\dagger - V^*[\chi^{22}, f]U^T)
\end{aligned}$$

In the single-particle basis, we can compute the interaction mean field  $\Gamma_{(1),ij} = \bar{V}_{ijkl}\rho_{(1),lk}$  and the pairing field  $\Delta_{(1),ij} = \frac{1}{2}\bar{V}_{ijkl}\kappa_{(1),kl}$ :

$$\begin{aligned}
\Gamma_{(1),ij} &= \bar{v}_{ijkl}\rho_{(1),lk} \\
&= i\bar{v}_{ijkl}\left(U_{l\alpha}[\chi^{11}, f]_{\alpha\beta}U_{\beta k}^\dagger + U_{l\alpha}(\chi^{12} - \{\chi^{12}, f\})_{\alpha\beta}V_{\beta k}^T \right. \\
&\quad \left. - V_{l\alpha}^*(\chi^{21} - \{\chi^{21}, f\})_{\alpha\beta}U_{\beta k}^\dagger - V_{l\alpha}^*[\chi^{22}, f]_{\alpha\beta}V_{\beta k}^T\right) \\
\Delta_{(1),ij} &= \frac{1}{2}\bar{v}_{ijkl}\kappa_{(1),kl} \\
&= \frac{i}{2}\bar{v}_{ijkl}\left(U_{l\alpha}[\chi^{11}, f]_{\alpha\beta}V_{\beta k}^\dagger + U_{l\alpha}(\chi^{12} - \{\chi^{12}, f\})_{\alpha\beta}U_{\beta k}^T \right. \\
&\quad \left. - V_{l\alpha}^*(\chi^{21} - \{\chi^{21}, f\})_{\alpha\beta}V_{\beta k}^\dagger - V_{l\alpha}^*[\chi^{22}, f]_{\alpha\beta}U_{\beta k}^T\right)
\end{aligned}$$

To clean up the presentation a bit, let us introduce the following:

$$\begin{aligned}
J_{ij\alpha\beta}^{11} &= i\bar{v}_{ikjl}U_{l\alpha}U_{\beta k}^\dagger & J_{ij\alpha\beta}^{22} &= -i\bar{v}_{ikjl}V_{l\alpha}^*V_{\beta k}^T \\
K_{ij\alpha\beta}^{12} &= i\bar{v}_{ikjl}U_{l\alpha}V_{\beta k}^T & K_{ij\alpha\beta}^{21} &= -i\bar{v}_{ikjl}V_{l\alpha}^*U_{\beta k}^\dagger \\
L_{ij\alpha\beta}^{12} &= i\bar{v}_{ijkl}U_{l\alpha}U_{\beta k}^T & L_{ij\alpha\beta}^{21} &= -i\bar{v}_{ijkl}V_{l\alpha}^*V_{\beta k}^\dagger \\
M_{ij\alpha\beta}^{11} &= i\bar{v}_{ijkl}U_{l\alpha}V_{\beta k}^\dagger & M_{ij\alpha\beta}^{22} &= -i\bar{v}_{ijkl}V_{l\alpha}^*U_{\beta k}^T
\end{aligned}$$

Then the fields simplify to

$$\begin{aligned}
\Gamma_{(1),ij} &= J_{ij\alpha\beta}^{11}[\chi^{11}, f]_{\alpha\beta} + K_{ij\alpha\beta}^{12}(\chi^{12} - \{\chi^{12}, f\})_{\alpha\beta} + K_{ij\alpha\beta}^{21}(\chi^{21} - \{\chi^{21}, f\})_{\alpha\beta} + J_{ij\alpha\beta}^{22}[\chi^{22}, f]_{\alpha\beta} \\
2\Delta_{(1),ij} &= M_{ij\alpha\beta}^{11}[\chi^{11}, f]_{\alpha\beta} + L_{ij\alpha\beta}^{12}(\chi^{12} - \{\chi^{12}, f\})_{\alpha\beta} + L_{ij\alpha\beta}^{21}(\chi^{21} - \{\chi^{21}, f\})_{\alpha\beta} + M_{ij\alpha\beta}^{22}[\chi^{22}, f]_{\alpha\beta}
\end{aligned}$$

Now we can transform the fields back into the quasiparticle basis:

$$\begin{aligned}
\mathcal{H}_1 &= \begin{pmatrix} U^\dagger & V^\dagger \\ V^T & U^T \end{pmatrix} \begin{pmatrix} \Gamma_1 & \Delta_1 \\ -\Delta_1^* & -\Gamma_1^* \end{pmatrix} \begin{pmatrix} U & V^* \\ V & U^* \end{pmatrix} \\
&= \begin{pmatrix} U^\dagger\Gamma_1U + U^\dagger\Delta_1V - V^\dagger\Delta_1^*U - V^\dagger\Gamma_1^*V & U^\dagger\Gamma_1V^* + U^\dagger\Delta_1U^* - V^\dagger\Delta_1^*V^* - V^\dagger\Gamma_1^*U^* \\ V^T\Gamma_1U + V^T\Delta_1V - U^T\Delta_1^*U - U^T\Gamma_1^*V & V^T\Gamma_1V^* + V^T\Delta_1U^* - U^T\Delta_1^*V^* - U^T\Gamma_1^*U^* \end{pmatrix}
\end{aligned}$$

Assuming further that the full matrix  $\chi$  is Hermitian, then  $\chi^{11*} = \chi^{11}$ ,  $\chi^{22*} = \chi^{22}$ , and  $\chi^{12*} = \chi^{21}$ . This leads in turn to

$$\begin{aligned}
[\chi^{11}, f]^* &= -[\chi^{11}, f] \\
[\chi^{22}, f]^* &= -[\chi^{22}, f] \\
(\chi^{12} - \{\chi^{12}, f\})^* &= (\chi^{21} - \{\chi^{21}, f\}) \\
(\chi^{21} - \{\chi^{21}, f\})^* &= (\chi^{12} - \{\chi^{12}, f\})
\end{aligned}$$

The whole mess written out is

$$\begin{aligned}
\mathcal{H}_{(1),ab}^{11} = & \left( U_{ai}^\dagger U_{jb} J_{ij\alpha\beta}^{11} + U_{ai}^\dagger V_{jb} \frac{M_{ij\alpha\beta}^{11}}{2} + V_{ai}^\dagger U_{jb} \frac{M_{ij\alpha\beta}^{11*}}{2} + V_{ai}^\dagger V_{jb} J_{ij\alpha\beta}^{11*} \right) (f_\beta - f_\alpha) \chi_{\alpha\beta}^{11} \\
& + \left( U_{ai}^\dagger U_{jb} J_{ij\alpha\beta}^{22} + U_{ai}^\dagger V_{jb} \frac{M_{ij\alpha\beta}^{22}}{2} + V_{ai}^\dagger U_{jb} \frac{M_{ij\alpha\beta}^{22*}}{2} + V_{ai}^\dagger V_{jb} J_{ij\alpha\beta}^{22*} \right) (f_\beta - f_\alpha) \chi_{\alpha\beta}^{22} \\
& + \left( U_{ai}^\dagger U_{jb} K_{ij\alpha\beta}^{12} + U_{ai}^\dagger V_{jb} \frac{L_{ij\alpha\beta}^{12}}{2} - V_{ai}^\dagger U_{jb} \frac{L_{ij\alpha\beta}^{21*}}{2} + V_{ai}^\dagger V_{jb} K_{ij\alpha\beta}^{21*} \right) (1 - f_\alpha - f_\beta) \chi_{\alpha\beta}^{12} \\
& + \left( U_{ai}^\dagger U_{jb} K_{ij\alpha\beta}^{21} + U_{ai}^\dagger V_{jb} \frac{L_{ij\alpha\beta}^{21}}{2} - V_{ai}^\dagger U_{jb} \frac{L_{ij\alpha\beta}^{12*}}{2} + V_{ai}^\dagger V_{jb} K_{ij\alpha\beta}^{12*} \right) (1 - f_\alpha - f_\beta) \chi_{\alpha\beta}^{21}
\end{aligned}$$

$$\begin{aligned}
\mathcal{H}_{(1),ab}^{12} = & \left( U_{ai}^\dagger V_{jb}^* J_{ij\alpha\beta}^{11} + U_{ai}^\dagger U_{jb}^* \frac{M_{ij\alpha\beta}^{11}}{2} + V_{ai}^\dagger V_{jb}^* \frac{M_{ij\alpha\beta}^{11*}}{2} + V_{ai}^\dagger U_{jb}^* J_{ij\alpha\beta}^{11*} \right) (f_\beta - f_\alpha) \chi_{\alpha\beta}^{11} \\
& + \left( U_{ai}^\dagger V_{jb}^* J_{ij\alpha\beta}^{22} + U_{ai}^\dagger U_{jb}^* \frac{M_{ij\alpha\beta}^{22}}{2} + V_{ai}^\dagger V_{jb}^* \frac{M_{ij\alpha\beta}^{22*}}{2} + V_{ai}^\dagger U_{jb}^* J_{ij\alpha\beta}^{22*} \right) (f_\beta - f_\alpha) \chi_{\alpha\beta}^{22} \\
& + \left( U_{ai}^\dagger V_{jb}^* K_{ij\alpha\beta}^{12} + U_{ai}^\dagger U_{jb}^* \frac{L_{ij\alpha\beta}^{12}}{2} - V_{ai}^\dagger V_{jb}^* \frac{L_{ij\alpha\beta}^{21*}}{2} + V_{ai}^\dagger U_{jb}^* K_{ij\alpha\beta}^{21*} \right) (1 - f_\alpha - f_\beta) \chi_{\alpha\beta}^{12} \\
& + \left( U_{ai}^\dagger V_{jb}^* K_{ij\alpha\beta}^{21} + U_{ai}^\dagger U_{jb}^* \frac{L_{ij\alpha\beta}^{21}}{2} - V_{ai}^\dagger V_{jb}^* \frac{L_{ij\alpha\beta}^{12*}}{2} + V_{ai}^\dagger U_{jb}^* K_{ij\alpha\beta}^{12*} \right) (1 - f_\alpha - f_\beta) \chi_{\alpha\beta}^{21}
\end{aligned}$$

$$\begin{aligned}
\mathcal{H}_{(1),ab}^{21} = & \left( V_{ai}^T U_{jb} J_{ij\alpha\beta}^{11} + V_{ai}^T V_{jb} \frac{M_{ij\alpha\beta}^{11}}{2} + U_{ai}^T U_{jb} \frac{M_{ij\alpha\beta}^{11*}}{2} + U_{ai}^T V_{jb} J_{ij\alpha\beta}^{11*} \right) (f_\beta - f_\alpha) \chi_{\alpha\beta}^{11} \\
& + \left( V_{ai}^T U_{jb} J_{ij\alpha\beta}^{22} + V_{ai}^T V_{jb} \frac{M_{ij\alpha\beta}^{22}}{2} + U_{ai}^T U_{jb} \frac{M_{ij\alpha\beta}^{22*}}{2} + U_{ai}^T V_{jb} J_{ij\alpha\beta}^{22*} \right) (f_\beta - f_\alpha) \chi_{\alpha\beta}^{22} \\
& + \left( V_{ai}^T U_{jb} K_{ij\alpha\beta}^{12} + V_{ai}^T V_{jb} \frac{L_{ij\alpha\beta}^{12}}{2} - U_{ai}^T U_{jb} \frac{L_{ij\alpha\beta}^{21*}}{2} + U_{ai}^T V_{jb} K_{ij\alpha\beta}^{21*} \right) (1 - f_\alpha - f_\beta) \chi_{\alpha\beta}^{12} \\
& + \left( V_{ai}^T U_{jb} K_{ij\alpha\beta}^{21} + V_{ai}^T V_{jb} \frac{L_{ij\alpha\beta}^{21}}{2} - U_{ai}^T U_{jb} \frac{L_{ij\alpha\beta}^{12*}}{2} + U_{ai}^T V_{jb} K_{ij\alpha\beta}^{12*} \right) (1 - f_\alpha - f_\beta) \chi_{\alpha\beta}^{21}
\end{aligned}$$

$$\begin{aligned}
\mathcal{H}_{(1),ab}^{22} = & \left( V_{ai}^T V_{jb}^* J_{ij\alpha\beta}^{11} + V_{ai}^T U_{jb}^* \frac{M_{ij\alpha\beta}^{11}}{2} + U_{ai}^T V_{jb}^* \frac{M_{ij\alpha\beta}^{11*}}{2} + U_{ai}^T U_{jb}^* J_{ij\alpha\beta}^{11*} \right) (f_\beta - f_\alpha) \chi_{\alpha\beta}^{11} \\
& + \left( V_{ai}^T V_{jb}^* J_{ij\alpha\beta}^{22} + V_{ai}^T U_{jb}^* \frac{M_{ij\alpha\beta}^{22}}{2} + U_{ai}^T V_{jb}^* \frac{M_{ij\alpha\beta}^{22*}}{2} + U_{ai}^T U_{jb}^* J_{ij\alpha\beta}^{22*} \right) (f_\beta - f_\alpha) \chi_{\alpha\beta}^{22} \\
& + \left( V_{ai}^T V_{jb}^* K_{ij\alpha\beta}^{12} + V_{ai}^T U_{jb}^* \frac{L_{ij\alpha\beta}^{12}}{2} - U_{ai}^T V_{jb}^* \frac{L_{ij\alpha\beta}^{21*}}{2} + U_{ai}^T U_{jb}^* K_{ij\alpha\beta}^{21*} \right) (1 - f_\alpha - f_\beta) \chi_{\alpha\beta}^{12} \\
& + \left( V_{ai}^T V_{jb}^* K_{ij\alpha\beta}^{21} + V_{ai}^T U_{jb}^* \frac{L_{ij\alpha\beta}^{21}}{2} - U_{ai}^T V_{jb}^* \frac{L_{ij\alpha\beta}^{12*}}{2} + U_{ai}^T U_{jb}^* K_{ij\alpha\beta}^{12*} \right) (1 - f_\alpha - f_\beta) \chi_{\alpha\beta}^{21}
\end{aligned}$$

Looking back to 4.9, we see that we can write it in the same form as 4.8:

$$\begin{aligned}
\frac{1}{2}\text{Tr}(\mathcal{H}_1\mathcal{R}_1) = & \bar{\mathcal{M}}''_{\alpha\beta ab}{}^{11,11}\chi_{\alpha\beta}^{11}\chi_{ba}^{11} + \bar{\mathcal{M}}''_{\alpha\beta ab}{}^{12,11}\chi_{\alpha\beta}^{12}\chi_{ba}^{11} + \bar{\mathcal{M}}''_{\alpha\beta ab}{}^{21,11}\chi_{\alpha\beta}^{21}\chi_{ba}^{11} + \bar{\mathcal{M}}''_{\alpha\beta ab}{}^{22,11}\chi_{\alpha\beta}^{22}\chi_{ba}^{11} \\
& \bar{\mathcal{M}}''_{\alpha\beta ab}{}^{11,12}\chi_{\alpha\beta}^{11}\chi_{ba}^{12} + \bar{\mathcal{M}}''_{\alpha\beta ab}{}^{12,12}\chi_{\alpha\beta}^{12}\chi_{ba}^{12} + \bar{\mathcal{M}}''_{\alpha\beta ab}{}^{21,12}\chi_{\alpha\beta}^{21}\chi_{ba}^{12} + \bar{\mathcal{M}}''_{\alpha\beta ab}{}^{22,12}\chi_{\alpha\beta}^{22}\chi_{ba}^{12} \\
& \bar{\mathcal{M}}''_{\alpha\beta ab}{}^{11,21}\chi_{\alpha\beta}^{11}\chi_{ba}^{21} + \bar{\mathcal{M}}''_{\alpha\beta ab}{}^{12,21}\chi_{\alpha\beta}^{12}\chi_{ba}^{21} + \bar{\mathcal{M}}''_{\alpha\beta ab}{}^{21,21}\chi_{\alpha\beta}^{21}\chi_{ba}^{21} + \bar{\mathcal{M}}''_{\alpha\beta ab}{}^{22,21}\chi_{\alpha\beta}^{22}\chi_{ba}^{21} \\
& \bar{\mathcal{M}}''_{\alpha\beta ab}{}^{11,22}\chi_{\alpha\beta}^{11}\chi_{ba}^{22} + \bar{\mathcal{M}}''_{\alpha\beta ab}{}^{12,22}\chi_{\alpha\beta}^{12}\chi_{ba}^{22} + \bar{\mathcal{M}}''_{\alpha\beta ab}{}^{21,22}\chi_{\alpha\beta}^{21}\chi_{ba}^{22} + \bar{\mathcal{M}}''_{\alpha\beta ab}{}^{22,22}\chi_{\alpha\beta}^{22}\chi_{ba}^{22}
\end{aligned} \tag{4.10}$$

#### 4.2.4 The Inertia Tensor

##### The total kinetic energy

Expressions 4.8 and 4.10 can be combined into one single expression involving the vector-like object  $\chi$  and the matrix-like object  $\bar{\mathcal{M}} = 2(\bar{\mathcal{M}}' + \bar{\mathcal{M}}'')$

$$E_{kin} = \frac{1}{2}\chi^\dagger \bar{\mathcal{M}} \chi \tag{4.11}$$

$$\chi_{\alpha\beta} \equiv \begin{pmatrix} \chi_{\alpha\beta}^{11} \\ \chi_{\alpha\beta}^{12} \\ \chi_{\alpha\beta}^{21} \\ \chi_{\alpha\beta}^{22} \end{pmatrix}, \quad \chi_{ab}^\dagger = (\chi_{ab}^{11*} \chi_{ab}^{12*} \chi_{ab}^{21*} \chi_{ab}^{22*})$$

$\bar{\mathcal{M}}$  is given by column in table 4.1, where it gets an entire page to itself because there's a whole lot of text.

Now we have an expression for the energy in terms of an inertia tensor  $\bar{\mathcal{M}}$  and the expansion parameter  $\chi$ . We already know that  $\chi$  is related to time-dependent changes in the density  $\dot{\mathcal{R}}_0$ ; now let us further try to relate  $\chi$  to changes in the collective shape multipole moments of the nucleus. You can use equations 4.5 or 4.6 to change variables to  $\dot{\mathcal{R}}_0$  instead of  $\chi$ , but I'm going to skip that for now because what we really want is to use  $\dot{q}$  and I'm running out of  $\mathcal{M}$ 's.

*Sanity Check:* As in the case of the ATDHFB equations from section 4.2.2, in the  $T = f = 0$  case, the  $^{11}$  and  $^{22}$  terms vanish completely in the lines leading up to 4.8 and 4.10 and we are left with familiar [zero-temperature] ATDHFB expressions. In

Table 4.1: The full FT-ATDHFB matrix, listed by column

$$\begin{aligned}
\bar{\mathcal{M}}_{1:1} &= \frac{1}{2} \begin{pmatrix} (E_b - E_a)(f_a - f_b)\delta_{\alpha\alpha}\delta_{\beta\beta} - (f_a - f_b) \left[ \bar{v}_{ikjl} \left( U_{ai}^\dagger U_{jb} U_{l\alpha} U_{\beta k}^\dagger - V_{ai}^\dagger V_{jb} U_{l\alpha}^* V_{\beta k}^T \right) + \frac{\bar{v}_{ijkl}}{2} \left( U_{ai}^\dagger V_{jb} U_{l\alpha} V_{\beta k}^\dagger - V_{ai}^\dagger U_{jb} U_{l\alpha}^* V_{\beta k}^T \right) \right] (f_\beta - f_\alpha) \\ (1 - f_a - f_b) \left[ \bar{v}_{ikjl} \left( U_{ai}^\dagger V_{jb}^* U_{l\alpha} U_{\beta k}^\dagger - V_{ai}^\dagger U_{jb}^* U_{l\alpha}^* V_{\beta k}^T \right) + \frac{\bar{v}_{ijkl}}{2} \left( U_{ai}^\dagger U_{jb}^* U_{l\alpha} V_{\beta k}^\dagger - V_{ai}^\dagger V_{jb}^* U_{l\alpha}^* V_{\beta k}^T \right) \right] (f_\beta - f_\alpha) \\ -(1 - f_a - f_b) \left[ \bar{v}_{ikjl} \left( V_{ai}^T U_{jb} U_{l\alpha} U_{\beta k}^\dagger - U_{ai}^T V_{jb} U_{l\alpha}^* V_{\beta k}^T \right) + \frac{\bar{v}_{ijkl}}{2} \left( V_{ai}^T V_{jb} U_{l\alpha} V_{\beta k}^\dagger - U_{ai}^T U_{jb} U_{l\alpha}^* V_{\beta k}^T \right) \right] (f_\beta - f_\alpha) \\ (f_a - f_b) \left[ \bar{v}_{ikjl} \left( V_{ai}^T V_{jb}^* U_{l\alpha} U_{\beta k}^\dagger - U_{ai}^T U_{jb}^* U_{l\alpha}^* V_{\beta k}^T \right) + \frac{\bar{v}_{ijkl}}{2} \left( V_{ai}^T U_{jb}^* U_{l\alpha} V_{\beta k}^\dagger - U_{ai}^T V_{jb}^* U_{l\alpha}^* V_{\beta k}^T \right) \right] (f_\beta - f_\alpha) \end{pmatrix} \\
\bar{\mathcal{M}}_{2:2} &= \frac{1}{2} \begin{pmatrix} -(f_a - f_b) \left[ \bar{v}_{ikjl} \left( U_{ai}^\dagger U_{jb} U_{l\alpha} V_{\beta k}^T + V_{ai}^\dagger V_{jb} V_{l\alpha} U_{\beta k}^T \right) + \frac{\bar{v}_{ijkl}}{2} \left( U_{ai}^\dagger V_{jb} U_{l\alpha} U_{\beta k}^T - V_{ai}^\dagger U_{jb} V_{l\alpha} V_{\beta k}^T \right) \right] (1 - f_\alpha - f_\beta) \\ (E_a + E_b)(1 - f_a - f_b)\delta_{\alpha\alpha}\delta_{\beta\beta} + (1 - f_a - f_b) \left[ \bar{v}_{ikjl} \left( U_{ai}^\dagger V_{jb}^* U_{l\alpha} V_{\beta k}^T + V_{ai}^\dagger U_{jb}^* V_{l\alpha} U_{\beta k}^T \right) + \frac{\bar{v}_{ijkl}}{2} \left( U_{ai}^\dagger U_{jb}^* U_{l\alpha} U_{\beta k}^T - V_{ai}^\dagger V_{jb}^* V_{l\alpha} V_{\beta k}^T \right) \right] (1 - f_\alpha - f_\beta) \\ -(1 - f_a - f_b) \left[ \bar{v}_{ikjl} \left( V_{ai}^T U_{jb} U_{l\alpha} V_{\beta k}^T + U_{ai}^T V_{jb} V_{l\alpha} U_{\beta k}^T \right) + \frac{\bar{v}_{ijkl}}{2} \left( V_{ai}^T V_{jb} U_{l\alpha} U_{\beta k}^T - U_{ai}^T U_{jb} V_{l\alpha} V_{\beta k}^T \right) \right] (1 - f_\alpha - f_\beta) \\ (f_a - f_b) \left[ \bar{v}_{ikjl} \left( V_{ai}^T V_{jb}^* U_{l\alpha} V_{\beta k}^T + U_{ai}^T U_{jb}^* V_{l\alpha} U_{\beta k}^T \right) + \frac{\bar{v}_{ijkl}}{2} \left( V_{ai}^T U_{jb}^* U_{l\alpha} U_{\beta k}^T - U_{ai}^T V_{jb}^* V_{l\alpha} V_{\beta k}^T \right) \right] (1 - f_\alpha - f_\beta) \end{pmatrix} \\
\bar{\mathcal{M}}_{3:3} &= \frac{1}{2} \begin{pmatrix} (f_a - f_b) \left[ \bar{v}_{ikjl} \left( U_{ai}^\dagger U_{jb} V_{l\alpha}^* U_{\beta k}^\dagger + V_{ai}^\dagger V_{jb} U_{l\alpha}^* V_{\beta k}^\dagger \right) + \frac{\bar{v}_{ijkl}}{2} \left( U_{ai}^\dagger V_{jb} V_{l\alpha}^* V_{\beta k}^\dagger - V_{ai}^\dagger U_{jb} U_{l\alpha}^* U_{\beta k}^\dagger \right) \right] (1 - f_\alpha - f_\beta) \\ -(1 - f_a - f_b) \left[ \bar{v}_{ikjl} \left( U_{ai}^\dagger V_{jb}^* V_{l\alpha}^* U_{\beta k}^\dagger + V_{ai}^\dagger U_{jb}^* U_{l\alpha}^* V_{\beta k}^\dagger \right) + \frac{\bar{v}_{ijkl}}{2} \left( U_{ai}^\dagger U_{jb}^* V_{l\alpha}^* V_{\beta k}^\dagger - V_{ai}^\dagger V_{jb}^* U_{l\alpha}^* U_{\beta k}^\dagger \right) \right] (1 - f_\alpha - f_\beta) \\ (E_a + E_b)(1 - f_a - f_b)\delta_{\alpha\alpha}\delta_{\beta\beta} + (1 - f_a - f_b) \left[ \bar{v}_{ikjl} \left( V_{ai}^T U_{jb} V_{l\alpha}^* U_{\beta k}^\dagger + U_{ai}^T V_{jb} V_{l\alpha}^* V_{\beta k}^\dagger \right) + \frac{\bar{v}_{ijkl}}{2} \left( V_{ai}^T V_{jb} V_{l\alpha}^* U_{\beta k}^\dagger - U_{ai}^T U_{jb} V_{l\alpha}^* U_{\beta k}^\dagger \right) \right] (1 - f_\alpha - f_\beta) \\ -(f_a - f_b) \left[ \bar{v}_{ikjl} \left( V_{ai}^T V_{jb}^* V_{l\alpha}^* U_{\beta k}^\dagger + U_{ai}^T U_{jb}^* V_{l\alpha}^* V_{\beta k}^\dagger \right) + \frac{\bar{v}_{ijkl}}{2} \left( V_{ai}^T U_{jb}^* V_{l\alpha}^* V_{\beta k}^\dagger - U_{ai}^T V_{jb}^* U_{l\alpha}^* U_{\beta k}^\dagger \right) \right] (1 - f_\alpha - f_\beta) \end{pmatrix} \\
\bar{\mathcal{M}}_{4:4} &= \frac{1}{2} \begin{pmatrix} (f_a - f_b) \left[ \bar{v}_{ikjl} \left( U_{ai}^\dagger U_{jb} V_{l\alpha}^* V_{\beta k}^T - V_{ai}^\dagger V_{jb} V_{l\alpha} V_{\beta k}^T \right) + \frac{\bar{v}_{ijkl}}{2} \left( U_{ai}^\dagger V_{jb} V_{l\alpha}^* U_{\beta k}^T - V_{ai}^\dagger U_{jb} V_{l\alpha} V_{\beta k}^T \right) \right] + (f_\beta - f_\alpha) \\ -(1 - f_a - f_b) \left[ \bar{v}_{ikjl} \left( U_{ai}^\dagger V_{jb}^* V_{l\alpha}^* V_{\beta k}^T - V_{ai}^\dagger U_{jb}^* V_{l\alpha}^* V_{\beta k}^T \right) + \frac{\bar{v}_{ijkl}}{2} \left( U_{ai}^\dagger U_{jb}^* V_{l\alpha}^* U_{\beta k}^T - V_{ai}^\dagger V_{jb}^* V_{l\alpha}^* V_{\beta k}^T \right) \right] (f_\beta - f_\alpha) \\ (1 - f_a - f_b) \left[ \bar{v}_{ikjl} \left( V_{ai}^T U_{jb} V_{l\alpha}^* V_{\beta k}^T - U_{ai}^T V_{jb} V_{l\alpha} V_{\beta k}^T \right) + \frac{\bar{v}_{ijkl}}{2} \left( V_{ai}^T V_{jb} V_{l\alpha}^* U_{\beta k}^T - U_{ai}^T U_{jb} V_{l\alpha} V_{\beta k}^T \right) \right] (f_\beta - f_\alpha) \\ (E_b - E_a)(f_a - f_b)\delta_{\alpha\alpha}\delta_{\beta\beta} - (f_a - f_b) \left[ \bar{v}_{ikjl} \left( V_{ai}^T V_{jb}^* V_{l\alpha}^* V_{\beta k}^T - U_{ai}^T U_{jb}^* V_{l\alpha}^* V_{\beta k}^T \right) + \frac{\bar{v}_{ijkl}}{2} \left( V_{ai}^T U_{jb}^* V_{l\alpha}^* U_{\beta k}^T - U_{ai}^T V_{jb}^* V_{l\alpha}^* U_{\beta k}^T \right) \right] (f_\beta - f_\alpha) \end{pmatrix}
\end{aligned}$$

essence, the rank of the problem reduces from dealing with a 4x4 matrix to dealing with a 2x2 matrix.

### Cranking Approximation

We already introduced the cranking approximation briefly in section 4.2.2 to simplify the relation between  $\chi$  and  $\dot{\mathcal{R}}_0$  when we assumed that changes in the density will have approximately no effect on the mean field ( $\mathcal{H}_1 \approx 0$ ). We can apply this to the energy expression, and then the inertia tensor is pretty simple:

$$\bar{\mathcal{M}} = \frac{1}{4} \begin{pmatrix} (E_b - E_a)(f_a - f_b) & 0 & 0 & 0 \\ 0 & (E_a + E_b)(1 - f_a - f_b) & 0 & 0 \\ 0 & 0 & (E_a + E_b)(1 - f_a - f_b) & 0 \\ 0 & 0 & 0 & (E_b - E_a)(f_a - f_b) \end{pmatrix} \quad (4.12)$$

### The Collective Shape Space

Suppose there is a set of collective variables  $(q_1, q_2, \dots, q_n)$  which describe changes in the density  $\mathcal{R}_0(t)$  at all times  $t$ . Then

$$\dot{\mathcal{R}}_0 = \sum_{\mu=1}^n \dot{q}_\mu \frac{\partial \mathcal{R}_0}{\partial q_\mu}$$

Relating this back to  $\chi$  using equations 4.6 (we'll just stick with the cranking approximation here) gives

$$\begin{aligned} \chi_{ab}^{11} &= \sum_{\mu=1}^n \frac{\hbar \dot{q}_\mu}{(E_a - E_b)(f_b - f_a)} \frac{\partial \mathcal{R}_{(0),ab}^{11}}{\partial q_\mu} \\ \chi_{ab}^{12} &= \sum_{\mu=1}^n \frac{\hbar \dot{q}_\mu}{(E_a + E_b)(1 - f_a - f_b)} \frac{\partial \mathcal{R}_{(0),ab}^{12}}{\partial q_\mu} \\ \chi_{ab}^{21} &= \sum_{\mu=1}^n \frac{\hbar \dot{q}_\mu}{(E_a + E_b)(1 - f_a - f_b)} \frac{\partial \mathcal{R}_{(0),ab}^{21}}{\partial q_\mu} \\ \chi_{ab}^{22} &= \sum_{\mu=1}^n \frac{\hbar \dot{q}_\mu}{(E_a - E_b)(f_b - f_a)} \frac{\partial \mathcal{R}_{(0),ab}^{22}}{\partial q_\mu} \end{aligned}$$

Of course, we should be careful here if the temperature is allowed to approach zero. In that case, then from equation 4.6 we see that  $\dot{\mathcal{R}}^{11} = \dot{\mathcal{R}}^{22} = 0$ . We should not have any  $\chi^{11}$  or  $\chi^{22}$  terms in the zero temperature case. The final form of the inertia tensor will also be affected. Likewise we should be careful not to divide by zero in the case of  $E_a = E_b$  as mentioned earlier at the end of section 4.2.2. Everything should work out fine since  $\chi^{11}$  and  $\chi^{22}$  are [potentially] finite numbers which are then multiplied by zero in the expression for  $\bar{\mathcal{M}}$ , but just be careful.

If we take this now and plug it into our energy expression 4.11 using the cranked inertia tensor 4.12, the following is what happens:

$$E_{kin} \approx \frac{1}{2} \sum_{\mu\nu} \dot{q}_\mu \dot{q}_\nu M_{\mu\nu} \quad (4.13)$$

where

$$M_{\mu\nu} = \frac{\hbar^2}{2} \left[ \frac{1}{(E_a - E_b)(f_b - f_a)} \left( \frac{\partial \mathcal{R}_{(0),ab}^{11}}{\partial q_\mu} \frac{\partial \mathcal{R}_{(0),ba}^{11}}{\partial q_\nu} + \frac{\partial \mathcal{R}_{(0),ab}^{22}}{\partial q_\mu} \frac{\partial \mathcal{R}_{(0),ba}^{22}}{\partial q_\mu} \right) + \right. \\ \left. \frac{1}{(E_a + E_b)(1 - f_a - f_b)} \left( \frac{\partial \mathcal{R}_{(0),ab}^{21}}{\partial q_\mu} \frac{\partial \mathcal{R}_{(0),ba}^{12}}{\partial q_\nu} + \frac{\partial \mathcal{R}_{(0),ab}^{12}}{\partial q_\mu} \frac{\partial \mathcal{R}_{(0),ba}^{21}}{\partial q_\mu} \right) \right] \quad (4.14)$$

In the zero temperature case, the first chunk (involving  $\mathcal{R}^{11}$  and  $\mathcal{R}^{22}$ ) should be replaced with zero.

### Perturbative cranking

Let's say you want to know the inertia at a single point on a PES, for instance, but you don't want to compute its neighbors in order to do a finite-differences derivative. Well, lucky for you there exist perturbative expressions for computing the inertia tensor at a single point. I'm not going to go through and show them here because they've already been done elsewhere (Nicolas' notes, for example), but I just wanted to mention it, along with a warning that they aren't always very good - especially, apparently, for triaxial shapes (see [23]).



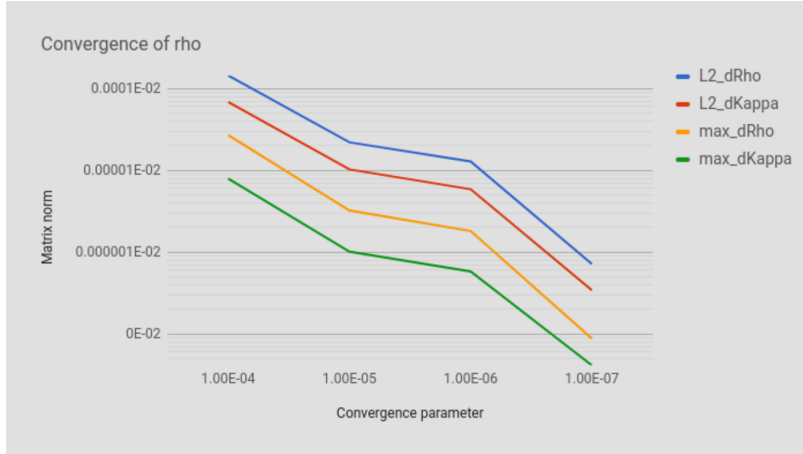


Figure 4.1: Shown are several different matrix norms for the matrix which is found by subtracting the density matrix of the last iteration from that of the second-to-last iteration. Specifically, these show results for the proton density  $\rho$  and the proton pairing density  $\kappa$  near the slightly-deformed ground state of  $^{240}\text{Pu}$ .

### 4.3 Numerical implementation

We run into some kind of issue when we try to implement 4.14 on a computer using small, non-zero temperatures (or, more generally, when  $f_b - f_a$  is small). I believe the primary source of the discrepancy is numerical, for the following reasoning:

It looks like the densities we compute in HFODD are probably accurate to within about 10% of the convergence parameter (I should do some additional testing to confirm this, but it seems plausible). That makes sense, because that's roughly the level of fluctuations we see in `E\_STAB` in the five iterations it takes for HFODD to declare the thing “converged”. So this means that we can't probably trust our densities to any precision greater than, roughly speaking, the convergence parameter.

So what does this mean for us? Specifically, what does this mean for our differentiation by finite differences with various sizes  $\delta q$ , and how does this change when we start dividing by our  $f_s$ ?

We might consider introducing a cutoff on the difference  $f_b - f_a$ . If we make our cutoff too tight, we start cutting off physics (the tail of the Fermi distribution). If we leave our cutoff too small, we start dividing by numbers that are smaller than the noise in the density matrix.

We know there is an ideal range of values  $\delta q$  to use when computing our derivative

using finite differences. Too large, and the derivative is unreliable; too small, and the we start crossing into more numerical regions. Suppose we take a value  $\delta q = 10^{-3}$  and set our HFODD convergence parameter to  $10^{-7}$ . Roughly-speaking, then, we would expect that we can set a cutoff for  $f_b - f_a$  of something around  $10^{-4}$  or so and still obtain reasonable results.

I did this with that  $^{240}\text{Pu}$  calculation for a few different cutoff values. To compare, I computed the exact  $T=0$  inertia. Then I computed the inertia using the same densities which had been computed at  $T=0$ , but introducing a fake temperature  $T=0.05$  to calculate the inertia.<sup>2</sup> The results are in table

Convergence	$10^{-7}$	
$\delta q$	$10^{-3}$	
Actual $T=0$ inertia:	1.585632E-02	
Cutoff	Inertia	% error
$10^{-4}$	1.585205E-02	-2.692933E-04
$10^{-5}$	1.585622E-02	-6.306634E-06
$10^{-6}$	1.585697E-02	4.099312E-05
$10^{-7}$	1.587771E-02	1.348989E-03
$10^{-8}$	1.612200E-02	1.675546E-02

...So I was a little off on my guess, but I think it illustrates my point.

## 4.4 Fission at finite temperature

There are several complications associated with considering a nucleus at finite temperature. I'd like to discuss first of all what that even means and why it is significant, and then I'll talk about some of the challenges of this approach.

The idea of considering fission as a finite temperature process stems from trying to develop a picture of induced fission. In induced fission, a neutron which carries some amount of energy is captured by a heavy nucleus in its ground state. That extra energy's gotta go somewhere, but where? In a large nucleus, you have all sorts of places, including any number of single particle excitations, or combination of single particle excitations, or perhaps the entire nucleus moves together as one large collective excitation. Apparently some people went through and did the combinatorics

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<sup>2</sup>I tried an actual  $T=0.05$  calculation, but it failed to converge and then I forgot about it

of these possible excitations and decided that the number of them was huge (like,  $\sim 10^{12}$  huge) [15]. So handling them explicitly just isn't going to work.

Additionally, DFT might not be the best tool for performing finite-temperature calculations. This is because DFT is typically implemented as a variational method, which means it's good for ground state calculations. But highly-deformed nuclei are inherently *not* in their ground state. In fact, this is true even for “zero-temperature” DFT as well. In practice the results we get are pretty good (most likely the system has time to equilibrate to its “deformed ground state” at each deformation step, or in other words the path to scission proceeds  $\sim$ adiabatically), but it's something to definitely keep in mind that (I suspect) could strongly affect your half-life predictions and fragment energies in particular. Furthermore, it's not clear to me how you might correct that should the need arise.

A third thing that Nicolas claims is that the temperature should depend on the actual deformation. I'm not sure where exactly this comes from but it sounds plausible to me.



# Chapter 5

## Nuclear Shape Deformations

Rick Casten has given several lectures about nuclear shape deformations and other such things. A lot of this will probably just be restating things he has said in my own words.

First of all, one important tool that you should understand in order to talk about nuclear shape deformations is a Nilsson diagram. First of all, you've seen level diagrams in atomic and nuclear spectroscopy. Figure 5.1, for instance, is a familiar illustration of low-lying energy levels for a harmonic oscillator potential, both before and after adding a spin-orbit interaction term which leads to the well-known nuclear "magic numbers."

Now imagine you stretch out the nucleus somehow. That'll certainly change the spacing and position of the energy levels, because some electron orbitals have a sort of intrinsic shape characteristic that might be better- or worse-suited for the new elongation.

Finally, imagine that you do the stretching *continuously*. That is what is done in a Nilsson diagram. For example, in figure 5.2, the system is elongated from a spherical ground state, and the changing energy levels are the curves, which frequently end up crossing one another. An important thing to notice is that, for different deformations you might have different shell gaps, and as well you might find that different orbitals are more favorable at different deformations.

Anyway, that's all helpful *once you know* the deformation. And there's a lot of useful and interesting things you can say and predict using a Nilsson diagram - heck, if you know the shape you can [qualitatively] even *draw* a Nilsson diagram, just by

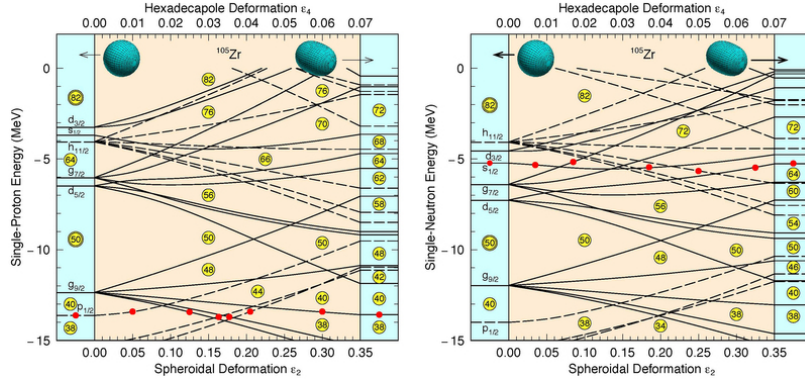


Figure 5.2: Nilsson Diagram for Zr-105, plotted against elongation parameter  $\epsilon_2$

thinking about the physical system and how the orbitals are probably behaving. BUT if you want to understand why a nucleus deforms in the first place, that's a whole other story.

## 5.1 What causes nuclear ground state deformations?

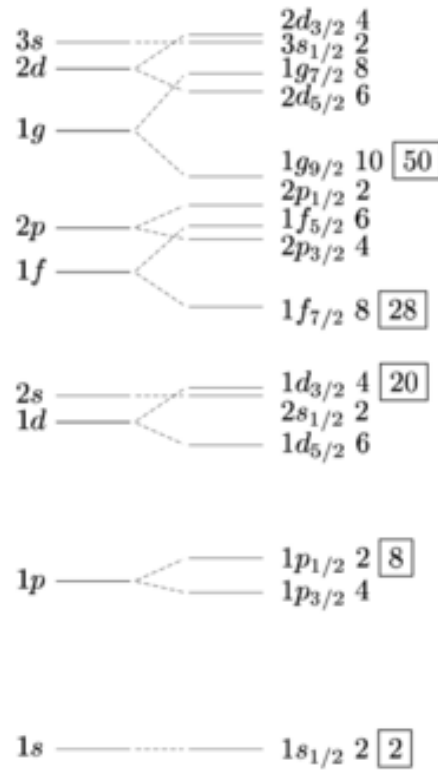
As with most peculiarities of nuclear structure, the source of nuclear deformation is primarily an artifact of shell structure. In particular, when there is a large shell gap, the nucleus will get sort of "locked" into a particular stable configuration, and if that happens to be a deformed configuration because of the orbital characteristics of the outermost nucleons (because that's the only thing that could matter, right?), then so be it.

A question that I have is how is there ground state deformation in even-even nuclei? Because even-even nuclei all have, without exception, spin-parity  $0^+$ , and yet  $^{152}\text{Dy}$  (for example) is highly-deformed. Am I misunderstanding the implications of such a spin-parity assignment? Or am I misunderstanding what is meant by "ground state deformed"?

I don't think this is a real answer, but one way to identify even-even deformed nuclei is to look for nuclei with a large  $\frac{E(4^+)}{E(2^+)}$  ratio (or a related method is to look for those with a relatively-small  $E(2^+)$ ).

## 5.2 Phenomenology of Nilsson Diagrams

[Basically here is where you were thinking about Casten's slides. He goes through and talks about whether a level's energy will go up or down, and how it will curve, just by thinking about the orbital motion of single particles around different axes of the deformed system.]



## 5.3 What causes nuclear ground state deformations? Part 2

### 5.3.1 What causes fission?

I think there's a couple of effects at play that lead to fission. First of all, what gets the nucleus moving in the first place, and second, what *keeps* it moving?

To answer the first question, imagine you were to buy a bunch of nucleons at the store and then put them in a box together. Just dump them in with some arbitrary configuration. They'll start to attract and repel one another and there will be kind of a chaotic mess of particle motions to keep track of. TDHF will kind of give you a sense of what's going on in sort of an average sense.

Figure 5.1: From Wikipedia: "Low-lying energy levels in a single-particle shell model with an oscillator potential (with a small negative l2 term) without spin-orbit (left) and with spin-orbit (right) interaction. The number to the right of a level indicates its degeneracy, (2j+1). The boxed integers indicate the magic numbers."

Eventually, the system might settle into a set of sort of normal modes. There

will probably be several overlapping normal modes happening at once, so the motion will still look pretty chaotic, but in some average sense you might get something that starts to move with some pseudo-regularity. And with time (I suppose regardless of whether the system motion is regular or not), the system might (for example) elongate, and in fact it might elongate enough for there to be a level crossing in the Nilsson diagram.

When this happens, the system has some deciding to do. It might continue on its current trajectory, or it might jump onto another trajectory (that is, there might be a nucleonic transition from one energy level to another). I suppose it is pretty difficult in practice for a nucleon to make these transitions, because you have all kind of things like conservation of angular momentum and Pauli's principle and such to consider. BUT if you transition a pair of nucleons instead of just one, you can skirt around a lot of these issues, and so I think that's what frequently tends to happen. That is why pairing correlations are sometimes called the "lubricant" of nuclear fission [8].

To go further brings you into the world of diabatic vs adiabatic level crossings. Witek talks about this in [19] (and that's what I'm trying to read through and understand right now). First, some terminology: The words "diabatic" and "adiabatic" come from Greek: "a" = "not", "dia" = "through", "batok" = "passable." So at a diabatic level crossing, the levels just pass right through one another without interacting or acknowledging one another. At an adiabatic level crossing, there might be some kind of level mixing as a result of residual interactions (basically, your single-particle picture wasn't good enough, I suppose). This is the point being illustrated in figure 1 of that reference: In the diabatic picture, you have two independent harmonic oscillators that happen to occupy the same space, whereas in the adiabatic picture, you have just a couple of messy, non-symmetric potential wells.

## 5.4 Between barrier and scission

I was asked a question during my second committee meeting by Filomena that is worth reflecting on: why can we use Langevin dynamics (which I believe is a semiclassical construction) to describe the pathway from barrier to scission? And I think the answer lies in the adiabatic approximation, that collective motion is slow compared



to single particle motion. That said, it merits some additional thought, perhaps once I get around to programming it.

I was talking with Samuel the other day, and we’re trying to figure out a better way to predict the fragments that doesn’t involve the large, multidimensional PES we’ve got for cases like plutonium and oganesson. The current framework for that requires you to have the action at each point along the outer turning line, and then the shape of the PES from the outer turning line to scission. We are lucky because 2-dimensions seems to be sufficient for describing the fragment distributions fairly well ( $Q_{20}$  and  $Q_{30}$ ). But still, is there a better way?

No matter what, we’ll probably need the barrier in order to find the action. Unless you can think of another way to compute the action as a function of where it leaves the barrier. So then instead you might try to find ways to avoid computing the PES way out there, instead. The approach used now is Langevin, which is really pretty much a classical description. Additionally, Andre Michaudon’s review in *Advances in Nuclear Physics Volume 6* suggests that properties near the ground state are dominated by shell effects, while structure properties for highly-deformed systems are mostly “washed-out by residual interactions” (there, they say, the LDM actually does a pretty good job).

What I’m wondering is the following: That highly-deformed case is pretty complicated because you don’t quite have a single hydrogen-like “central mean-field” (like you would near the ground state) and you don’t quite have two of them, either (like you would post-scission). Instead you have some messy in-between thing, with crazy mixed-up orbitals, and really since there is no central force, you just have a jumbled bunch of loose particles gettin’ in each others’ fields and no<sup>1</sup> clear order, flowing back and forth until the clusters move too far away from one another and you’re left with whatever’s left. So your best bet to model that is probably some kind of statistical model. That’s why Langevin is used; you need something basically with a temperature dependence.

A question worth asking is: are thermal fluctuations all you need there? Or do you need to include quantum fluctuations somehow as well? Because I don’t know

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<sup>1</sup>Clearly there must be some order, because the fragments that leave are clearly correlated with the shape of the parent

if Langevin handles both. And my other [related] question is: does the shape of the PES really matter after that? Does it somehow still include whatever effects of shell structure are important there? Or were those only important to get you through the barrier, and now thermal physics will carry you to scission along whatever trajectory they were already on, and all the important shell information is already baked in? I'm guessing you still need some type of shell structure to guide you, or somehow to build that quantum information into your dispersion. So the way it works now is that quantum mechanics builds the playground for you, and then you let thermal physics play around and do whatever it wants, but the rules are it has to play on the ground you built for it.

What if you just built your quantum mechanical interaction into the Langevin equations as an additional force term? Like including a Skyrme term in there or something? Would that preserve all the information you need? Or maybe there's another, similar framework to work in? Or perhaps there's another framework that allows you to handle the fluctuations after the barrier. By then, I feel like you've done sort of the hard part - I mean, there's two hard parts: the 1st half, and the 2nd half, but you get what I mean. By then, I should say, you've tunneled through the barrier. You've taken the system from a point where it is primarily quantum mechanical and brought it to a point where it is primarily thermal, and now it has to go back from thermal to quantum mechanical. To put it another way, you took it from one starting point to a lot of midpoints, and now you have to take it from a lot of midpoints to a relatively small number(?) of end points. I wonder if, at this point, you'd be able to hijack any of the Hauser-Feshbach work that has been done.

Another, totally unrelated question that might be worth addressing is: Does tri-axiality ever play a role near scission?

## 5.5 Describing Scission

(This is probably way out of place, but whatever...) Intuitively, you might think that the driving factor which determines fragment ID distributions would be shell structure of the fragments. And if I'm reading this right [17, 2nd paragraph + references], you'd be partly right: the *real* driving factor is shell structure of the *prefragments*, and an

important factor in understanding this is that the prefragments are typically highly-deformed, which means that their shell structure is probably totally different than it would be for those same fragments in their ground state.

## 5.6 Multipole moments

Something I have said in the past is that the multipole moments of a system are essentially related to the spherical harmonics expansion. That's true-ish, but I should do this a little bit more carefully.

Imagine you have a single particle, and origin, and a coordinate system. Furthermore, suppose for the sake of argument that the origin does not coincide with the location of the particle. Automatically, then, the system has some dipole moment. This moment is a geometrical attribute of the system. It contains information about the charge of the system and the way it is distributed. The sum of multipole moments gives the total potential.

But in fact you might go further, for if the particle is not aligned with a coordinate axis, then you introduce higher-order multipole moments, as well. In general it will have a monopole contribution, a dipole contribution, a quadrupole contribution, etc. Griffiths E&M p. 147-148 shows how this can be done systematically, as does Jackson p. 145. When you draw out a system involving an origin, a source point, and an observation point, and you describe the relation between them using some law of cosines stuff, and expand out in terms of  $\frac{r'}{r}$ , where  $r'$  is the distance from origin to source point and  $r$  the vector separating origin and observation points, then you end up getting Legendre polynomials. That is given for a single source point in Griffiths (3.94), and then you can sum over all source points as seen in Griffiths (3.95). Jackson uses an expansion in spherical harmonics  $Y_l^m$  instead of Legendre polynomials  $P_l$ , which I supposed contains fundamentally the same information but going back and forth takes some work (see Jackson (4.2)). The multipole moment is defined explicitly and plainly in Jackson in terms of spherical harmonics. It is the part that contains strictly the information about the source, and which is independent of the observation point:

$$\begin{aligned}
\Phi(\vec{x}) &= \frac{1}{4\pi\epsilon_0} \int \frac{\rho(\vec{x}')}{|\vec{x} - \vec{x}'|} d^3x' \\
&= \frac{1}{\epsilon_0} \sum_{l,m} \frac{1}{2l+1} \left[ \int Y_l^{*m}(\theta', \phi') r'^l \rho(\vec{x}') d^3x' \right] \frac{Y_l^m(\theta, \phi)}{r^{l+1}} \\
&\equiv \frac{1}{\epsilon_0} \sum_{l,m} \frac{1}{2l+1} q_{lm} \frac{Y_l^m(\theta, \phi)}{r^{l+1}}
\end{aligned}$$

I'm not quite sure what the “charge” is in the multipole decomposition of the nuclear shape, but maybe it's the number of nucleons? Or even just 1? I just base that on the fact that the total monopole moment for protons equals the number of protons (so if you compute the monopole moment for each particle individually, I don't know what they will be individually, but together they'll add up to the total number of protons). Actually, as I think about it, it's probably just the mean field density. That's the main thing we're using/looking for, after all. Duh.

So the main thing you need to get out of this (regardless of how we got there; multipole moments are standard now) is that multipole moments are defined in the following way:

$$q_{lm} = \int Y_l^{*m}(\theta', \phi') r'^l \rho(\vec{x}') d^3x'$$

As far as HFB is concerned, your multipole constraint appears with a Lagrange multiplier:  $\hat{H} - \lambda \hat{N} - \lambda_i \hat{Q}_i$ . The  $\hat{Q}$  is the multipole operator. What is it operating on? The density. I don't know if that coefficient has any physical significance.

On a related note, sometimes nuclear deformations are described in terms of the coordinates  $(\beta_{20}, \gamma)$  instead of  $(Q_{20}, Q_{22})$ . There's some kind of relation between  $\beta_2$  and  $Q_{20}$ , and I'm not positive what it is but [14] has an equation

$$\beta_{20} = \frac{\sqrt{20\pi}}{5A} \frac{Q_{20}}{r^2}$$

where  $r = 1.2A^{\frac{1}{3}}$  fm. I don't know if that's generally true but I'ma hold onto it for a while and see if anything else comes up.

In fact, a slightly more general definition (which I found in [2]) is the following:

$$\begin{aligned}
Q_{20} &= \int d^3r \rho(r) (2z^2 - x^2 - y^2) \\
Q_{22} &= \int d^3r \rho(r) (x^2 - y^2) \\
\beta_2 &= \sqrt{\frac{5}{16\pi}} \frac{4\pi}{3AR_0^2} \sqrt{Q_{20}^2 + Q_{22}^2} \\
\gamma &= \arctan \sqrt{2} \frac{Q_{22}}{Q_{20}}
\end{aligned}$$

where again  $R_0 = 1.2A^{\frac{1}{3}}$  fm.

A question you might consider asking at some point is whether there are reasonable conditions under which seemingly-pedantic cases where, for instance,  $Q_{22} = 0$  but triaxiality is intact, might occur.



# Chapter 6

## Some notes on HFODD

Since a big chunk of my time has been spent wrestling with the DFT solver HFODD and digging around the source code and whatnot, I thought it would be a good idea to write out at least some of the useful things I’ve learned that should make it easier for others (or myself) down the line.

First of all, a note on the structure of the code: The actual “solver,” or the main function that makes up the skeleton of HFODD only goes to about line 8918 or so in the main file (depending on which version of the code you are using, of course; this figure refers to the Argonne SVN `branches/inertia` version of the code as of 23 August 2017, for whatever that’s worth). A better way to identify it might be to look for the subroutine `PROANG`, and the main function ends right before that. And actually, the Hartree-Fock iterations don’t actually begin until  $\sim 3820$ , and end  $\sim 8365$ ; everything before tends to be setup and reading in data and whatnot; everything after is mostly writing data to files.

In fact, it takes a couple hundred more lines of setup inside the loop before any calculations are done, starting with the words “`CALCULATING THE MATRIX ELEMENTS OF THE NEUTRON MEAN FIELD`” and a call to `INTEGH` (which just adds the individual pieces together, apparently; it doesn’t really perform any matrix multiplications). Likewise, it then calculates the neutron pairing field (the matrix elements of the mean-field Skyrme Hamiltonian; multipole constraints are added in there via a call to `INTCON`). It mixes the HFB matrix, saves the fields, and then diagonalizes the HFB Hamiltonian (`HFBSI*` in the HO basis, where `*` depends on symmetries requested by the user). Then it does `QUABCS`, which calculates the new Fermi energy, followed by a

subroutine (for example, `CANQUA`) which finds and stores the U and V matrices, which transform between canonical and quasiparticle basis. That’s another 300 lines. And so what does it do after that? Well, it spends some time computing single-particle average properties (but only when it is “absolutely necessary”). **Then** it computes the Skyrme-functional densities and currents (`DENSHF`), the neutron density matrix, and from there, energies, magnetic moments, the RMS radius, and other properties of the system. That’s all done by about line 5000, and then it changes to protons. So it’s about 1000 lines of actual HFB calculations for neutrons and about another 1000 for protons (and even less than that, because some of those 1000 lines are just using the computed densities to compute other things). I guess that’s not surprising; it’s just building and diagonalizing a matrix. Everything else is seeing what cool things you can do with this thing you’ve just built.

The mean-field matrix diagonalization is completed by  $\sim 5985$ ; everything else inside the loop is just bonus physics calculations that take advantage of the newly-computed densities, with some error handling thrown in there as well. So don’t be too intimidated by the massive size of the code base; the actual functionality - everything you need to know about the code - is only around 9000 lines (still a lot, but nothing compared to the 200,000 or so lines that make up the entirety of HFODD).

Another thing to note is that there is by default a constraint on  $Q_{20}$ . There are, of course, plenty of preset values, but this one seems particularly obnoxious. I think there’s a way around it but I don’t remember off the top of my head what it was.  $\rightarrow$  I think you can set the stiffness parameter to zero.

In the table of energies, the so-called “total energy” (the very last term in the bottom right) is (so far as I can tell) given by equation I-9 (from the original HFODD paper; see also eq VI-96):

$$E_{tot} = E_{kinetic} + E_{Skyrme} + E_{Coulomb} + E_{pair} \quad (6.1)$$

$$+ [E_{LN} + E_{pot} + E_{Gog} + E_{Yuk} + E_{CM} + E_{rot}] \quad (6.2)$$



## Notes on specific subroutines, variables, etc. that I once found useful to know

Subroutine `paipri` appears to be printing values it got from the replay file. It uses the variable `EFER2X` internally, but it is called with `EFER2N`.

The record file is actually read in 3447, after some info is printed (`INFPRI`).

`ADJBAS` adjusts to find the optimal basis, given the requested value of  $Q_{20}$ .

`QMULCM` updates Lagrange multipliers of multipole constraints.

`QCNTRS` calculates energy contributions due to multipole constraints.

`INTCON` Calculates multipole moment constraining fields. Called inside `INTEGH`, which is where matrix elements of the Skyrme mean field are calculated (see eqn 28 of [10]). Returns `HPPCON`/`HPMCON` (or `HAUXPP`, `HAUXPM` as given in the subroutine call).

`INTEGH` Calculates mean-field Hamiltonian matrix elements. I believe, but am not positive, that this is eqn 26 in [10]. Nothing complicated is really computed in this subroutine; rather, it makes calls to a bunch of subroutines, which individually calculate the different pieces of things found in eqns 27-30, 111, etc, and then just adds the results into a single matrix.

`DENSHF` Calculates densities (see eqns 40-51 in [10])



# Chapter 7

## Nuclear Clusters

Today I'm trying to read and learn what I can about so-called "clusters." It doesn't sound to me like an inherently difficult concept, but apparently there are some things related to cluster formation that are poorly-understood, and besides that I want to see if I can better improve my study habits by basically keeping a "study journal." So here goes...

My introduction to clustering came from a line in a paper by Nicolas [26], where he refers to a small channel in the potential energy surface for  $^{240}\text{Pu}$  corresponding to something called "cluster radioactivity."

It comes up quite a bit more with a lot more references in Chunli's first localization paper [35]. The rest of Chunli's paper doesn't go into much more detail about what clusterization *is*, but it describes a technique for observing shell structure in clusters (or anything, really), even within a "smeared-out" DFT framework. It's cool because DFT tends to blur and spread out the impact of single-particle wavefunctions across the entire nuclear volume, but this localization technique gives you a way to see something shell-like within the nucleus. That's especially useful in fission because the formation of fragments is driven by the shell structure of the pre-fragments (and not the final fragments themselves). So if you start to see shell structure appearing in your scissioning nucleus, you might be able to say something about what the final fragments are, just based on the shell structure of the pre-fragments.

But I'm still skeptical.  $^{86}\text{Kr}$  and  $^{84}\text{Se}$  will probably have almost identical shell structure (magic  $N = 50$  for neutrons, and an off-shell even number of protons). Is it really likely that you'd be able to identify the different isotopes just using the localiza-

tion measure? I actually tested something very much like this back for platinum-176. There I actually used an even more extreme example of  $^{84}\text{Se}$ ,  $^{82}\text{Se}$ , and  $^{86}\text{Zr}$ . The seleniums were almost identical (the neutron spatial localization was only very slightly different), and the zirconium was even *pretty* similar (whatever that means). You can see the results somewhere on my computer where I have them stored, and I also showed a few sample figures in the `research_notes.tex` file, under **Nucleon Localization Function** → **28 September 2017**

But I digress...

Apparently historically, the idea of cluster emission was originally characterized by situations where the emitted fragment was larger than an alpha particle, but capped off at about  $Z_e^{\text{max}} = 28$  (see the introduction to [34] for kind of a historical overview of cluster radiation). However, starting in around 2012 and taking into account results from heavy and superheavy systems, the criteria was relaxed to allow for  $Z_e > 28$ . They had noticed that very often the larger remaining fragment was  $^{208}\text{Pb}$  or one of its neighbors, and so now cluster emission includes heavy fragments up to  $Z_e^{\text{max}} = Z - 82$  (see [20]). Physically, it's basically the same thing happening (lead sheds whatever is left and the rest forms a cluster); the only major difference is that superheavy isotopes can produce heavier clusters. Several models have been proposed to describe the phenomenon, such as suprasymmetric fission or tunneling of a preformed fragment through a potential barrier. We actually have a bit of useful information we can use to test that. If you look in my `research_notes.tex` file, under **Nucleon Localization Function** → **29 September 2017** you can see some nice diagrams that show the development of shell structure in the fragments of  $^{294}\text{Og}$ . Based solely on this set of results, I don't feel comfortable with the idea of a preformed fragment tunneling through a potential barrier - at least not for the smaller fragment. Look at the proton localization for krypton and you'll see that its shell structure doesn't develop until fairly late. The lead develops fairly quickly, however, and I believe that was the conclusion reached in [34].

Michal Warda gave a[n unpublished] presentation in September 2017 about cluster radioactivity in superheavy nuclei. He showed some cool pictures of potential energy surfaces evolving from actinides to superheavies, and you can totally see cluster emission go from a very unlikely branch to perhaps the dominant fission channel.

Ultimately his conclusions are:

- Asymmetric fission in superheavy nuclei region has the same nature as cluster radioactivity in actinides
- This decay may be dominant in some superheavy nuclei
- Sharp fragment mass distribution with  $^{208}\text{Pb}$  fragment is predicted

Cluster formation in actinides generally seems to be associated with a fairly long half-life (typically  $10^{11} - 10^{26}$  seconds, according to Warda’s presentation; see also [21] and references therein) and a low branching ratio relative to  $\alpha$  decay ( $10^{-9} - 10^{-16}$ ). However, he also shows a drastic reduction in the size of the barrier to cluster formation, from upwards of 25 MeV down to around 5 MeV, and I suspect the half-lives will see a major reduction as a consequence. It’s impossible to say for sure without actually *doing* the calculation, but I suspect just from looking at the barrier that it’ll be comparable with asymmetric fission in actinides or shorter. Figure 4 in [21] makes it look like  $\alpha$  decay will win out over cluster radioactivity only *just barely*, with a half-life only perhaps a factor of 10 shorter.

Also worth noting is that “Several attempts to detect  $^{12}\text{C}$  radioactivity of the neutron deficient  $^{114}\text{Ba}$  with a daughter in the neighborhood of the double magic  $^{100}\text{Sn}$ , predicted to have a larger  $b_\alpha$ , have failed” [21]. So it seems to be a phenomenon linked to lead or, more likely, heavy and superheavy elements. Seeing that for superheavy elements, cluster emission and asymmetric fission appear to be one and the same, it makes sense to think of cluster emission as a particularly asymmetric instance of regular, garden-variety fission.

## A note about “clusters”

The notion of a “cluster” is not, so far as I can tell, rigorously-defined. In all I’ve said leading up to this, cluster radiation/cluster emission is the process by which lead (or some lead-like nucleus) sheds its excess nucleons, and whatever is left just forms into its own so-called “cluster.” So in that case, a cluster is just a clump of leftover nucleons.

But as I say, that is not totally rigorous. Bastian and Witek published a paper (I should say, they *submitted* a paper, because at the time I am writing this, it is

only available on the arXiv: <https://arxiv.org/abs/1710.00579>) where they discussed “cluster formation in pre-compound nuclei.” Their argument was that entrance channel effects can’t necessarily be ignored in various collisions involving compound nuclei, because sometimes the nucleus isn’t as thermalized as we’d like to think (we haven’t lost all the information about the incoming particles).  $\alpha$  particles in particular like to stick together and move around in clumps. So in that case, “clusters” refers to substructures within the overall system (like  $\alpha$  particles hanging out at the tips of an elongated nucleus, or rings of carbon-12 forming near the middle).

There’s probably no real need to overthink this: “cluster” is just a useful word that describes organized nuclear structures which are smaller than the overall system under consideration. I don’t think anyone means anything more than that. Or at least, they probably shouldn’t.

## Alpha Clustering

An interesting question that hasn’t been immediately obvious to me is how to deal with the concept of alpha clusters. I don’t see a channel on my PES corresponding to an alpha decay. Perhaps it might manifest itself as a very narrow, deep channel that doesn’t show up with the resolution of my current oganesson surface. So I wanted to see what else people had come up with to predict alpha decay half-lives, and especially to see if there was anything more than just phenomenological hand waving. And it turns out the answer is yes. From what I understand, alpha decay (at least according to this thesis and the papers cited therein: <http://uir.unisa.ac.za/bitstream/handle/10500/1220/dissertation.pdf>) involves  $p-p$  and  $n-n$  pairs forming in high-lying states near the surface, with  $p-n$  pairing giving the final catalyst to let a particle shed off (configuration mixing).

## Remaining questions

Since localizations can be used to visualize clusters, I’m going to posit a question here (which was originally suggested by Gregory Potel): Would it be possible to visualize pairs, and not just individual nucleons? If so, it might be interesting to see how pairs move around as you near scission (perhaps especially as part of a time-dependent calculation).

# Chapter 8

## Bayesian Inference

A lot of my notes on statistical inference are in my UQ class notes from Fall 2017 with Mohsen Z, but I have some more fundamental questions that I'd like to understand and I think writing down insights as they come will ultimately prove helpful.

### 8.1 Bayes' Theorem

Let's say you have a model of some system, but you don't know the coefficients or parameters of the model. But you do have a bunch of data, and you'd like to use that data to go back and figure out what the model parameters probably are. For instance, in a coin toss, you might have a model like  $H(f) = \alpha * f$ , where  $f$  is the number of flips and  $H$  is the number of heads. You've done the experiment a hundred million times and you want to use your data to come up with some estimate for the coefficient  $\alpha$  (and perhaps even an uncertainty). You might also have some inkling of what that coefficient should be - for sure you know that it will be somewhere between 0 and 1, but maybe you have reason to believe that it's even somewhere in the interval  $[0.37, 0.54]$ , or that coin-flipping coefficients are manufactured around a normal distribution centered about 0.53.

The essence of Bayes' Theorem says that if you fold together everything that you know (your data) with what you suspect (your "prior"), then you can update your suspicion (your "posterior," which can in turn become a prior in your next round of estimation) to give you something probably better. Depending on the "forcefulness" of your prior, or the amount of data you've collected, you might see that the data

completely overwhelms the prior, or vice versa.

The prior could be anything from a flat line (if you have no idea what to expect) to a delta function (though I wouldn't recommend using that since it makes your posterior also a delta function unless you know for a fact what to expect, but then why are you even doing this?).

The likelihood is where you work your data in. An example likelihood function might involve an exponential of a chi-squared function, for example ( $P(D|H) \sim \exp(-\frac{\chi^2}{2})$ ). This would give some sort of distribution that is peaked at the “best fit” set of parameters. In general, a likelihood tells you “How likely was this outcome, given these parameters?” whereas the posterior tells you “How likely are these parameters, given the outcome?”

[These StackExchange questions has some helpful discussion:

<https://stats.stackexchange.com/questions/58564/help-me-understand-bayesian-prior-and-posterior-distributions>

<https://stats.stackexchange.com/questions/2641/what-is-the-difference-between-likelihood-and-probability>]

## 8.2 Markov Chain Monte Carlo

Let's say we have a set of data  $D$  and a model hypothesis with parameters  $H$ . Then Bayes' Theorem in this case might look like:

$$P(H|D) = \frac{P(D)P(D|H)}{P(H)} \quad (8.1)$$

Just for the sake of argument, our prior and likelihood might take the following forms:

$$\begin{aligned} P(D) &\sim \exp\left[\frac{1}{2}(\vec{x} - \vec{x}_0)^T C_p^{-1}(\vec{x} - \vec{x}_0)\right] \\ P(D|H) &\sim \exp\left[-\frac{\chi^2}{2}\right] \\ \chi^2 &= \sum_i \left[ \frac{\sigma^{th}(\vec{x}) - \sigma^{exp}}{\Delta\sigma} \right]^2 \end{aligned}$$

Maybe we want to estimate the sample distribution for the parameter  $x_1$ . We could do that essentially by integrating the posterior over all other parameters:



$$P(H_1|D) = \int P(D)P(D|H)dx_2dx_3\dots dx_n \quad (8.2)$$

In principle, this makes sense. You get a nice-looking one-dimensional distribution of values of  $x_1$  as sort of a histogram. In practice, though, that integral is probably really hard to solve. So instead you can turn to a method called Markov Chain Monte Carlo. In there, you pick a starting point in your sample space, and then you just do sort of a random walk (described by your Markov Chain). You take a bunch of steps, and you keep the ones that satisfy a set of conditions <sup>1</sup>. From these saved/logged/archived steps, you can put together essentially a histogram that represents the posterior distribution for that parameter.

“But Zachary!” you might ask. “If you’re only keeping points that give an improved ratio, then won’t you converge quickly to the ‘true’ value, and not have much to show in the tails?” And the answer is “not necessarily.” It might be that your prior is way out in the tails, for instance, and so your random walk might heavily favor those values at first until you have enough data to override. Or perhaps you’re in a weird saddle/local minimum of your multidimensional space where improving one parameter requires you to reduce the quality of another. Or perhaps you have a complicated, ill-posed, non-linear model where converging to the “true” parameter (which doesn’t really even exist in Bayesian statistics, but let’s pretend) might not immediately converge to the true value ( $\lim_{x \rightarrow x_{true}} \sigma^{th}(x) \neq \sigma^{exp}$  over some range of  $x$ ).

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<sup>1</sup>You’ll probably evaluate the prior and likelihoods at the old step and the new step, compute their ratio, and only keep the point if the ratio  $\frac{newpoint}{oldpoint} > 1$



# Chapter 9

## UQ for Nuclear DFT

### 9.1 Introduction

A recent goal in nuclear physics has been to develop models with quantified uncertainties (I wonder - where did that push start? Was it within the theory community? A request from experimentalists? A mandate from the funding sources?). One of these models - DFT - is useful all across the nuclear landscape. A recent collaboration sought to develop a UNiversal Energy Density Functional - hence the name of the collaboration, UNEDF. This family of three energy density functionals was designed to be applied across the entire nuclear chart, and each member of the set had a particular focus in mind: UNEDF0 was a proof of concept, UNEDF1 was optimized for large nuclear deformations, and UNEDF2 is designed to effectively capture the physics of shell structure. Furthermore, these functionals were designed with UQ in mind; each functional has an evaluated covariance matrix, and sensitivity analyses were performed for each of the parameters.

### 9.2 Compiling a list of uncertainties

So far I'm just brainstorming by outlining essentially every possible source of error or uncertainty I can think of in the physical model and its numerical implementation. At each step I'll discuss both some short- and long-term suggestions for ways to improve the outcome.

### 9.2.1 Nuclear Force

- We don't really *know* the nuclear force, per se... (my understanding is that it's just a residual interaction from the QCD interaction of the constituent quarks)
- Skyrme, Gogny, etc
- EDF parameterization
- EDF fitting strategy
- Coulomb...
- The mean-field approximation, and consequently, the pairing interaction - or in other words, correlations that go beyond just the mean-field
- ...

### 9.2.2 DFT Solver

I should mention here that there is some brief discussion at the beginning of the very first HFODD paper about different numerical techniques that can be (and perhaps *have been*) used to solve the HF(B) equations, such as finite-difference or conjugate gradient methods (see also subsection 7.3.3 of Ring and Schuck).

- Basis size - number of states, shells
- Basis type
- Integration mesh
- Determining convergence - That's hard to quantify exactly; it may be that we converge to a local, but not global minimum.
- Calculation of  $V_{eff}$  (subtracting off zero-point energy?)
- The whole thing about using a ground state-based method to calculate highly-deformed nuclei
- ...

### 9.2.3 Inertia

- Recipe for calculating (perturbative vs. nonperturbative, ATDHF vs GCM)
- Adiabatic approximation - “slow” collective motion
- Finite difference spacing
- Cutoff parameter (for finite temperature)

Here there’s a divergence which determines what comes next

### 9.2.4 Half-life, Pathway to Fragments

- Validity of WKB approximation
- Semi-classical SF half-life approximation
- Parameters determining frequency of tunneling attempts
- Interpolation of potential energy surface
- Choice of collective coordinates
- Choice of  $E_0$
- Identification of scission line
- Identification of least-action path inside the barrier (Dynamic programming method vs. Ritz method [vs. static least-energy path])
- Effectiveness of Langevin description of dynamics outside the barrier
- ...

## 9.3 Review of the DFT error analysis survey article [27]

There are two schools of thought when it comes to DFT, apparently. One is ... I’m not totally sure what the distinction is, actually. The first has something to do with

building a self-consistent mean-field (and my impression is that’s done *from scratch*, in some sense.) The other (which is what I’m familiar with) starts with a rather phenomenological potential (perhaps a Skyrme interaction), as opposed to one built from the ground up. Then you somehow come up with a set of parameters to tweak that Skyrme interaction. That’s where the UNEDF project takes off.

Essentially what this paper tries to do in the end, though, is to discuss the three types of uncertainties that can affect your DFT calculation results. There are numerical errors, which are pretty easy to understand and likewise to quantify. For example, in an iterative scheme, you can increase the number of iterations and see how the convergence of your solution is affected. Or if your calculation depends on a basis expansion, you can try running the calculation with different basis sizes and seeing what happens. As a general rule of thumb, if you want to quantify numerical errors, it’s probably just a matter of increasing the number of iterations/increasing the size of the basis/using a finer mesh. Nothing too mysterious here.

Harder to quantify is the effect of your theoretical model itself. Intuitively we believe that a DFT calculation should give better results than a liquid drop model calculation, or ab initio potentials will be superior to phenomenology, but it doesn’t always work out that way and oftentimes (if you’re extrapolating your model) it’s impossible to quantify. We assume that our description of the nucleus will be incomplete whenever we use a Skyrme-based potential, but we don’t really know *how* incomplete. And it’s not obvious how to go about determining that, short of just comparing against experiment (but again, you really have to be able to tease out your numerical error and your fitting bias). That’s why it would be nice to have either potentials, or at least coupling constants derived somehow from theory, and not just fit to data. Because if you can fit your coupling constants from theory, then at least you know what approximations it took to get from “exact” to “approximate.” So a good question to answer would be “How could we get from the basic NN-interaction to Skyrme?” Is such a thing even possible? Skyrme is phenomenological, but maybe it could emerge from an analytic NN interaction somehow? If only we had an analytic form for a NN interaction (or even approximation that was analytic)...

But wait - isn’t that what Skyrme *is*? Oh gosh, we’re hosed...

Anyway, the other thing to quantify here is the uncertainty in your model param-

eters. These are separate from the shortcomings of the model itself - you accept that your model is off by some amount, because of what you might consider a systematic error in your model (a missing bit of physics, for instance). Already you can see how hard it is to tease apart your model uncertainty and your model parameter uncertainty, because what we're about to ask you to do is to find the exact parameters to an inexact model. What would that even mean? So maybe you settle for a "best" set of parameters. Okay, fine. Still tough to do "exactly." For one thing, your fit will depend on the numerical implementation of the model (all that stuff about basis size, number of iterations, grid spacing, etc again applies, plus maybe some assumptions made in the solver that restrict it to a certain subset of the full model). Then it also depends on the optimization scheme you use (least squares fitting or something else). And finally, it depends on the experimental data you feed into it. In fact, there have been a few studies aimed at understanding the impact of different types of data on your final results (a few are mentioned towards the end of section 4.1, and there is also the paper done by Jordan, Nicolas, Witek, and others [9]).

These points are supplemented with some examples from the UNEDF project, showing how difficult it can be to tease apart the different sources of uncertainty but trying anyway. They talk a bit about the Bayesian problem they solved to do the fitting, and then about some of the assumptions they made in order to compute the covariance matrix and such, and tried to argue whether those assumptions were reasonable or not. To really understand what was done beyond these illustrative introductions, though, I imagine I'll need to look back at the original papers. So next stop: UNEDF0!

## 9.4 Review of the UNEDF0 paper [16]

Something cool about this, right off the bat after reading the abstract, is that they gained "new physics insights...by the advanced covariance analysis."

There's a nice brief review of some of the other parameter-fitting schemes that have been attempted. Those are nice because they help to understand better the nature of parameter-fitting uncertainties.

In practice, the way things worked was to take their DFT solver and compile or

run it inside a wrapper code (POUNDERS, I believe) that took care of the statistics part, and called on the DFT solver whenever it needed something.

The first thing they did was they tried to find, for as many parameters as possible, a sensible range of values in which to do a parameter search. The EDF terms are not directly-related to any observable quantities; however, the equation of state for infinite nuclear matter can be recast both in terms of observable quantities as well as Skyrme functional densities and coupling constants, and from there we can draw an approximate relation between the two. Then, since we have a rough idea of what the equation of state physical quantities of interest/scale are, we have a good starting place for our parameter search.

Then a set of experimental data was chosen to represent the chart of nuclides as a whole. This set has been published as a standard set of data for model calibrations, to reduce the uncertainty related with choice of experimental data.

## 9.5 Review of “Error Estimates of Theoretical Models: a Guide” [11]

## 9.6 Miscellaneous

This paper (<https://e-reports-ext.llnl.gov/pdf/790483.pdf>) has a nice table (Table 2) which shows the impact that your input starting points have on your final solution, even using the same algorithm and the same data points. That’s very interesting, actually, because in most cases, the difference between starting and ending points have the same sign, and the starting and ending points almost have the same rough magnitudes between functionals.

This paper (J. Phys. G: Nucl. Part. Phys. 42 (2015) 034031) does more-or-less the same thing.

I don’t have a section on chiral EFT, but an essential idea from that, which I learned from a Dick Furnstahl talk, is that if you can identify a scale in your expansion, then in nice systems (like relativity or presumably chiral EFT), your coefficients will be of roughly the same order, which means you can estimate truncation errors with some confidence.



# Chapter 10

## HFB, DFT, and Beyond Mean-Field Corrections

Beyond mean-field corrections are used to include correlations which are discarded or distorted through the HFB/SCMF formalism. Some of these may deal with configuration mixing and collective motion, and these are treated using the Generator Coordinate Method. Other corrections are used to impose symmetries which are found in nature but which are violated in the mean-field calculation. I am going to explain these latter beyond mean-field correction in the context of Lipkin-Nogami, which is used to compensate for the loss of particle-number conservation due to the Bogoliubov transformation. There are, as I will mention later, other such corrections one can make, such as a rotational correction to restore good angular momentum, for instance. For more, one can read p.15 of Nicolas Schunck's and Luis Robledo's review article on fission [29], or especially section III-B of Michael Bender, et al's review article on self-consistent mean-field models [7].

### Lipkin-Nogami

The Lipkin-Nogami method of restoring particle number symmetry to the nucleus involves splitting the energy density into two terms:

$$\mathcal{E}_{TOT} = \mathcal{E}_{HFB} + \mathcal{E}_{LN}$$

where  $\mathcal{E}$  is computed as

$$\mathcal{E}_{LN} = -\lambda_2 (\langle N^2 \rangle - N^2) = -2\lambda_2 \text{Tr} \rho (1 - \rho)$$

Lipkin-Nogami is an example of a beyond mean-field correction. Beyond mean field corrections are used to restore symmetries which are otherwise broken in the HFB equations, such as particle number conservation, a good angular momentum number (rotational invariance correction), or parity. Once the HFB solution is obtained, the conserved quantity is restored (in principle) by projecting your solution back onto the space of solutions with good quantum numbers. In principle, this projection should be done before variation (VAP), so that the wavefunctions from which the variational principle draws are only those which have the correct symmetries. However, VAP methods are quite challenging. You can approximate the effect by swapping the order (PAV). Here you take whatever solution successfully minimizes the HFB equations and then project *that* onto the space of “good” wavefunctions. It’s easier sometimes than VAP and may get you close, but of course it is not guaranteed that you’ll get the correct answer.

Sometimes even pure PAV is too hard, and you might want a simpler, more “phenomenological” way of guessing the effect of VAP. You do your mean-field HFB calculation, get some answer  $|\Psi\rangle$ , and then use some formula to estimate what the effect of VAP *would have* been on your variational energy, had you done it that way. This is what Lipkin-Nogami is for particle number restoration. You solve the HFB equations at the mean field level, and instead of properly projecting your states onto states with good particle number symmetry, you calculate a correction term to your energy to estimate the effect that proper projection would have had. You can calculate the particle number variance  $\langle \Delta \hat{N}^2 \rangle$  just from your densities, and there is a recipe for calculating  $\lambda_2$  from your density as well (see eqn 92 of Bender, et al, Rev Mod Phys 75 (2003), or see how it is implemented in HFODD below). In this case, since you are not actually using Lipkin-Nogami to do particle number restoration (even approximately), then the Lipkin correction term to the energy is not physical. The number you want, and which you actually have available, is the original mean-field solution *without* any beyond mean-field corrections (or, I mean, you can add other ones, but just know that the “default” energy HFODD is giving you is including a Lipkin energy which is not a correct beyond mean-field correction to the energy).

Worth mentioning is the fact that, at least in HFODD, the Lipkin-Nogami term is included as part of the variational energy. So you aren't minimizing with respect to the pure HFB energy, but rather the pure HFB energy PLUS the Lipkin-Nogami correction term. Hopefully you appreciate this distinction, and understand that it can have an effect on the overall properties of your system.

In your 4D oganesson calculation (and in Jhila's paper about pairing correlations in fission), you do something just a little bit different. You aren't doing Lipkin-Nogami, but you do something similar, but for a completely different purpose. Here you fix the value of  $\lambda_2$ . By doing so, you effectively impose that particle number variance will have a certain "importance" to the system: higher  $\lambda_2$  means that particle number fluctuations are more important to your system than if you had a smaller  $\lambda_2$ . Since this correction term to your energy is included in the variation, then you are baking this preference into your solution. And since large particle number fluctuations are tied to stronger pairing, then by imposing a large value of  $\lambda_2$  you are indirectly imposing a large pairing strength ( $V_0$ ) into your system (and this in turn manifests itself through a larger pairing gap  $\Delta$  and a larger pairing energy).

In HFODD,  $\lambda_2$  is evaluated on every iteration using the updated densities from the previous iteration, starting from some initial value you can set in the input. It is also possible in HFODD to fix the value of lambda and not update it for each new iteration, if you're into that kind of thing. It is given approximately via the seniority-pairing interaction by

$$\lambda_2 = \frac{G \text{Tr}(1 - \rho) \kappa \text{Tr} \rho \kappa - 2 \text{Tr}(1 - \rho)^2 \rho^2}{4 [\text{Tr} \rho (1 - \rho)]^2 - 2 \text{Tr} \rho^2 (1 - \rho)^2}$$

where

$$G = G_{eff} = -\frac{\bar{\Delta}^2}{E_{pair}}, \quad E_{pair} = -\frac{1}{2} \text{Tr} \Delta \kappa, \quad \bar{\Delta} = \frac{\text{Tr} \Delta \rho}{\text{Tr} \rho}$$

The UNEDF functionals included pairing strengths for both protons and neutrons as part of the Skyrme parameter set when they were optimizing, so the pairing strength is actually given as a parameter instead of computed from the densities in (for example) HFODD ← Double-check this! But I think that's how it'll work? I'm getting lost in the source trying to find out... (4-19-2017) But definitely you shouldn't use Lipkin-Nogami with the EDF UNEDF1-HFB. That was explicitly computed *with-*

out Lipkin-Nogami. You could set the lambdas all you want but they won't do a darn thing, unless you turn on Lipkin-Nogami but that'd be dumb because then you'd get the wrong answer.

## Unresolved questions

Aside from not really knowing how GCM or GOA work, I also don't quite understand why it is that symmetry-restoring corrections apparently tend to lower the total energy. The way I'm seeing it now is (at least for PAV): you have a solution which minimizes your HFB energy, and it is some linear combination of wavefunctions which may or may not have the correct symmetries. So you project out the ones that aren't helping and only keep the ones with good quantum numbers. And somehow this should lower your overall energy? I mean, unless you're like averaging the energy over wavefunctions, and somehow the wavefunctions with good quantum numbers have the lowest energy. Then by cutting out the others you'd allow your average to settle into that lowest value. And in reality, I suspect the truth is something like that - maybe not averaging, of course, but it might make sense that the states with good quantum numbers are optimized for the Hamiltonian density you started with, which has a symmetry-restoring-on-the-average term. So I dunno. Am I barking up the wrong tree?

## Functionals for odd-mass nuclei

This is admittedly not a beyond-mean field concept, but it is in some sense beyond the standard mean field calculations I'm used to.

There are I suppose four ways to fit a functional to odd-mass nuclei/time-odd terms:

- Derive the functional from a force (Skyrme, for instance. This is more in line with SkM\* than UNEDF)
- Impose local gauge invariance
- Landau parameters (See Osterfield 1992, with a 2018 PRL involving Remco Zegers for an update)

- Ignore the time-odd terms altogether.

These ideas are discussed in PRC 81 024316 by Schunck et al (<https://doi.org/10.1103/PhysRevC.81.024316>).

## Single-reference vs. multi-reference HFB

Another not-necessarily beyond-mean-field concept that I'm going to discuss here is the notion of single-reference vs multi-reference HFB. What you're used to is single-reference, and so far as I can tell that name comes about because you calculate everything with respect to a single Slater determinant - the vacuum state. GCM is a multi-reference extension of what you're familiar with. The foundation of GCM is that you construct a wavefunction that is a coherent superposition of different HFB states, as opposed to just a single one.

There is an analog within EDF theory - MR-EDF vs SR-EDF. Essentially there you're just dealing with density matrices instead of wavefunctions, but you already know how that goes.

See [http://www.int.washington.edu/talks/WorkShops/int\\_13\\_1a/People/Bender\\_M/Bender\\_M.pdf](http://www.int.washington.edu/talks/WorkShops/int_13_1a/People/Bender_M/Bender_M.pdf).

## Convergence of HF/HFB iterations

A question I've wondered about is how do we have any kind of assurance that our HFB iterations will even converge? Like, we diagonalize the matrix and use the result to construct a whole new problem. Who's to say that the solution to this entirely-new problem will be anywhere even close to the original problem/solution? And it turns out that is exactly true. I mean, you've already had plenty of cases where a bad initial guess led to a chaotically diverging result (or some other kind of divergence), so you're already aware that convergence isn't guaranteed. But I wanted to know more! And it turns out, so did someone else on the internet. Here's a stackexchange post about exactly this: <https://scicomp.stackexchange.com/questions/1297/why-does-iteratively-solving-the-hartree-fock-equations-result-in-convergence>

Not only do they answer the question ("No, convergence isn't guaranteed"), but they also manage to provide some conditions under which convergence *is* guaranteed, and furthermore they give some algorithms and tools that help encourage convergence.

In case the link ever breaks, here are the two best answers:

Answer #1

The Hartree-Fock equations are the result of performing constrained Newton-Raphson minimization of the energy with respect to the parameter space of Slater determinants (I don't have my copy of Szabo-Ostlund at hand, but I believe this is pointed out in the derivation). Hence, HF-SCF will converge if your starting guess is in a convex region around a minimum. Elsewhere, it may or may not converge. SCF convergence fails all the time. answered Feb 13 '12 at 12:54 Deathbreath

The impression I am getting is that the SCF method only converges if (i) the function is well behaved and (ii) the initial guess occurs sufficiently near the global minimum. Would you agree with this? – James Womack Feb 14 '12 at 11:28

It need not be near the global minimum. For instance, you might be trapped in a symmetry with a local minimum that isn't global. If the function is ill-behaved, I agree that you will most likely not converge. I encourage you to derive the gradient and the Hessian of the HF energy functional w.r.t. the orbital coefficients yourself and compare them to the Fock matrix. Nocedal's book on optimization is great for understanding the convergence behavior in this light then. – Deathbreath Feb 14 '12 at 13:01

Even if you're near a minimum, you can still have problems with systems that have closely spaced minima or low-curvature potential surfaces. In particular in my experience, systems like actinide (and I assume lanthanide) compounds with near-degenerate levels and states around the minimum tend to be difficult, since your optimiser can repeatedly overshoot the actual minimum. (Which is where damping comes in handy.) – Aesin Feb 14 '12 at 20:15

Answer #2

Density functional theory (DFT) also uses a one-particle approach similar to Hartree-Fock, although the effective potential is a little more involved.

To achieve a global minimum, the problem is approached as a non-linear fixed point problem which, as Deathbreath said, can be solved via a constrained Newton-Raphson minimization. A common approach in the DFT community is to use Broyden's Method which if organized correctly (J Phys A 17 (1984) L317) requires only two vectors: the current input and output. (See Singh and Nordstrom, p. 91-92, for a quick overview of this method, or Martin, Appendix L, for a more complete overview of related techniques.) A more recent technique used in Wien2k attempts to overcome convergence difficulties with the Broyden method by employing a multi-secant method.(PRB 78 (2008) 075114, arXiv:0801.3098) answered Feb 13 '12 at 16:55 rcollyer

Another approach other than using quasi-Newton methods (Broyden) would also be DIIS. – Deathbreath Feb 13 '12 at 18:38





# Chapter 11

## The Fission Process

Describing fission is a multistep process. Nicolas showed a great figure (Fig 11.1) during his talk at a recent meeting about neutron star mergers that illustrates an overview of the fission process, including the inputs, observables, and intermediate steps that theorists use to build models.

The scope of my PhD has been in the pink region, limited to the case of spontaneous fission. This means that for an entrance channel, we take for granted the spherical (or nearly-spherical) ground state of a nucleus, and then proceed to do calculations in order to predict lifetimes and primary fission yields. A schematic overview of how this is done in our approach is shown in figure 11.2. In the adiabatic approximation, it is assumed that large-scale collective motion is much slower than the internal motion of individual nucleons. It is further assumed that a fissioning nucleus can be described via its large-scale collective motions - that is, by its shape.

Those assumptions in place, the process is broken into two parts: a tunneling part, in which the nucleus passes quantum mechanically through a region of shape space which is classically forbidden; and a dissipative part, in which the now-deformed nucleus evolves semiclassically towards scission, when the neck connecting the two fragments breaks.

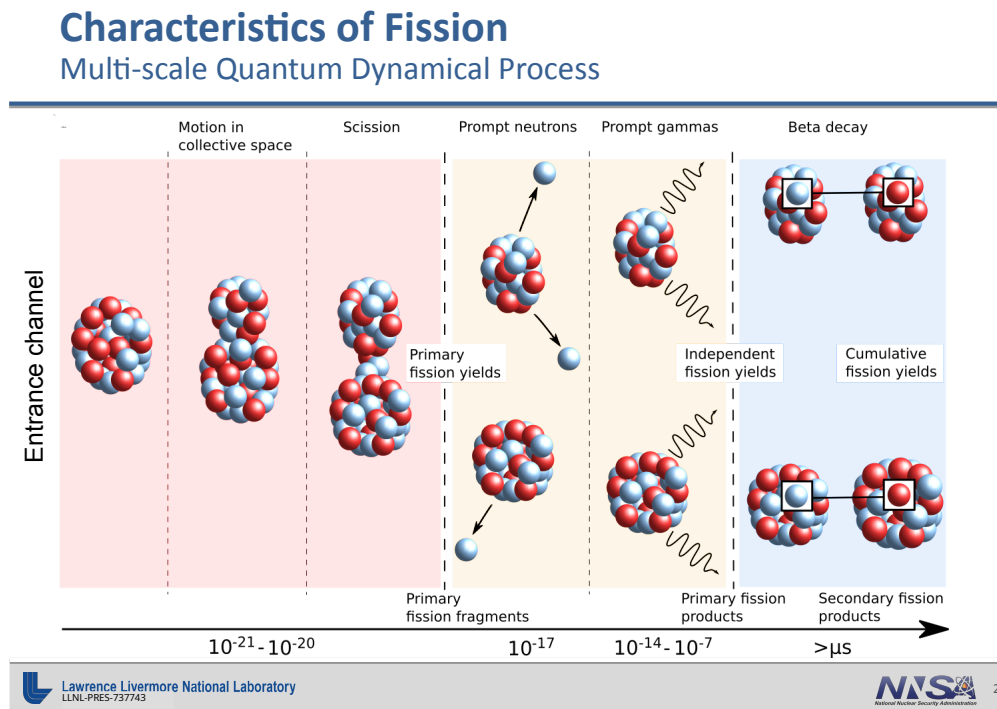


Figure 11.1: Overview of different steps of the fission process. Each step represent essentially a separate domain for theorists, with outputs from one domain/step serving as inputs for the next. So far, there is no comprehensive model of fission that describes the entire process from start to finish. (From a talk by Nicolas Schunck 19 July 2018)

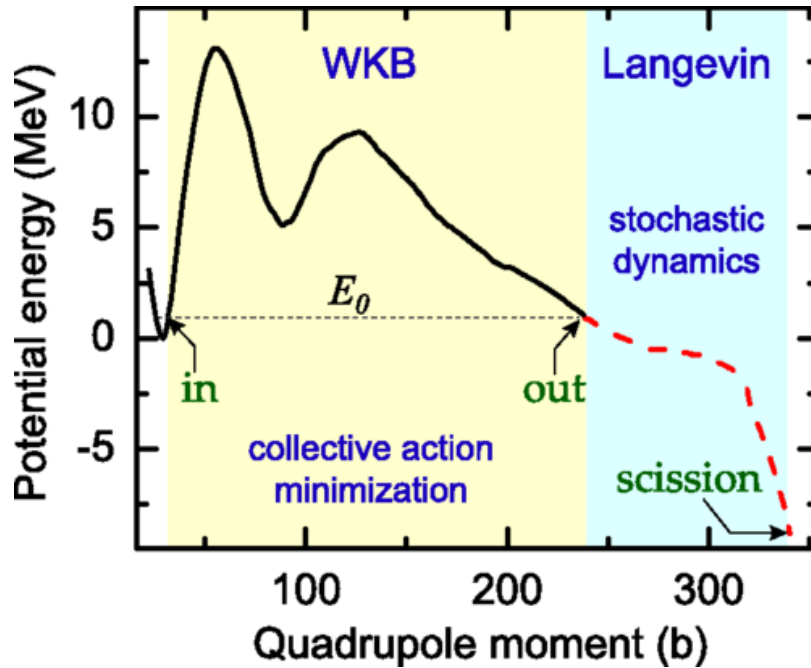


Figure 11.2: Schematic overview of our approach to fission, with a tunneling portion described via the WKB approximation, and dissipative dynamics described with the Langevin equations. Figure from [24].

## 11.1 Tunneling

### 11.1.1 What causes the peaks and valleys in the PES?

My understanding is that the peaks and valleys in a PES are related to the single-particle level densities. Regions of the PES with large shell gaps (be they spherical or deformed) will have valleys, while the intermediate regions don't have that energy lowering mechanism. This is based on my reading of [33].

## 11.2 Semiclassical dissipative motion

After emerging through the barrier, the nucleus is now highly-deformed but otherwise in a classically-allowed region of the potential-energy surface. At this point the nucleus is highly-unstable, and shell effects of the prefragments drive the nucleus toward scission. However, fluctuations within the nucleus will introduce some dissipation(?) into the system which will affect the yields. The framework which can describe these fluctuations is Langevin dynamics.

The Langevin equations used to approximately describe, for instance, motion of a particle inside a viscous fluid.

$$\frac{dp_i}{dt} = -\frac{p_j p_k}{2} \frac{\delta}{\delta x_i} \mathcal{M}_{jk}^{-1} - \frac{\delta V}{\delta x_i} - \eta_{ij} \mathcal{M}_{jk}^{-1} p_k + g_{ij} \Gamma_j(t) \quad (11.1)$$

$$\frac{dx_i}{dt} = \mathcal{M}_{ij}^{-1} p_j \quad (11.2)$$

Here the  $\eta_{ij}$  term describes dissipation (like friction or viscosity), while the  $\Gamma_j$  term represents a random force. The strengths of the dissipative and random force terms are related via the fluctuation-dissipation theorem:  $\sum_k g_{ik} g_{kj} = \eta_{ij} k_B T$ .

The essence of the fluctuation-dissipation theorem states that if there is some dissipative process (for instance, a particle moving in a fluid exerts drag, which converts kinetic energy to heat), then there corresponds a “reverse” process caused by thermal fluctuations (in our example, hot molecules in the fluid bump into the particle and cause it to move). I suppose that in equilibrium of a closed system there will be a constant back-and-forth between energy being dissipated through some process and thermal fluctuations reversing the process. In a scissioning nucleus, what would this look like?

Can we be sure that detailed balance is satisfied, and consequently that Langevin applies? I ask because Wikipedia reports that sometimes Spontaneous Symmetry Breaking can violate the assumptions needed for detailed balance.

The papers Jhilmam cites in [24] are [13] and [1]. In reading [13], he mentions a couple of review articles (his references 21 by Hilscher and Rossner and 22 by Hofmann) in which attempts to derive transport equation coefficients (your Langevin coefficients) are performed in a microscopic framework.

The friction coefficient should be related to the strength of the coupling between collective and intrinsic degrees of freedom. If that coupling is represented as a form factor  $f(R)$  where  $R$  represents a collective coordinate, then the friction strength goes as (according to equation 21)  $(f'(R))^2$ . This form factor is often assumed to be directly proportional to the collective coordinate  $f(R) \propto R$ , so the friction coefficient is constant. Without fluctuations, friction will always act to remove collective energy from the system, and transfer it to excitation energy  $E^*$ . The total energy  $E = E_{coll} + E^*$  will be constant.

The intrinsic motion is modeled in [13] as a collection of non-interacting harmonic oscillators. Perhaps if we used some actual nuclear structure input with n-particle, n-hole excitations we could make Langevin much more realistic! But I can only imagine that the computational complexity would shoot up drastically - you'd have to do a detailed levels calculation at *every single* deformation. Plus you'd still need to identify a suitable form for your collective-to-internal motion form factor. I have my doubts that there is a reasonable and straightforward way to do that.

If we assume that the intrinsic motion of single particles is uncorrelated, and if the mean energy of a given particle is  $T$  by the equipartition theorem (for a 1D oscillator), then we get the strength of the Gaussian term  $\Gamma_j$  via the expression that appears in [24], as well as the fluctuation-dissipation theorem which relates the strength of fluctuations to the dissipation. A small caveat is that the temperature is not constant in our case, since the heat bath is just the internal motion of the particles. If we assume that the “equilibration time” of the internal system is sufficiently small, then the consequence of this changing temperature is that the Langevin fluctuation strength coefficient is not constant. This is probably a safe bet for fission, which is a relatively-slow process, but not so much in deep inelastic scattering. We account for this non-constant temperature by setting  $T = \sqrt{E^*/a}$ , where  $a$  is a level density parameter (the so-called Fermi gas relation).

I suspect there's a way to extract some kind of energy from out of the Langevin equations - maybe one corresponding to an internal energy absorbed due to friction, and another collective energy. I don't suppose they might have a connection to the resulting fragment energies? Would the energies you extracted even be meaningful, since they don't contain quantum interaction energies or Coulomb repulsion of the fragments? I dunno...

## 11.3 Is adiabaticity a valid assumption?

I think it is pretty-well agreed that adiabaticity is more-or-less valid within the barrier itself. Potential energy surfaces do a good job of predicting distribution peaks and half-lives and so on. But as we already know, this static assumption seems to have trouble going between the tunneling portion to scission. Experimentally, this process

is very fast, like maybe on the order of  $10^{-21}$ s or so. I can't remember exactly what the time scale of single particle motion is, but I suspect it's not too far off. So maybe adiabaticity isn't such a good idea here.

"But why did Jhiliam's Langevin idea seem to work?" It did a pretty good job, to be sure, and it makes a lot of sense. But as we're seeing right now from the localizations and the inertia, it seems to perhaps be the case that the prefragments are actually pretty-well determined at the outer turning point. The tails come from those random statistical fluctuations, but generally-speaking it doesn't seem so much that the topology of the PES/collectivity of the system is the main thing here. I bet we'd get the correct peaks if we calculated the yield from the localizations right on the OTL, and the tails if we added some small fluctuations somehow, without reference to the PES between there and the scission line. I think it's possible there might be some other process at play, which depends more heavily on the single-particle motion than the collective motion. This is called, at least in the case of some PhD thesis I found by LiawJyeR1976(?), the "statistical theory of nuclear fission." At his time of writing in 1976, he says it wasn't clear which approach (adiabatic vs. not) was superior, and his references 12,18,19 discuss more about these I suppose (such as by Fong).

12. See the latest compilation on Nuclear Fission by Vandenbosch, R., and Huizenga, J. R. 18. Swiatecki, W. J., IAEA Proc. Symp. on Physics and Chemistry of Fission, Salzburg, Vol. I, 3 (1965). 19. Fong, P., Statistical Theory of Nuclear Fission, Gordon and Breach, Science Publishers, New York (1969). Also see Ignatyuk, A. V., Sov. J., Nucl. Phys., 9, 208 (1969).

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