

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

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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.

BCS Theory and HF+BCS ([?, ?])

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 [?]).

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 wave-functions, 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 $|BCS\rangle = \prod_{k>0} (u_k + v_k a_k^\dagger a_{\bar{k}}^\dagger) |0\rangle$, 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 wavefunctions $a_k^\dagger |0\rangle$, 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 [?], for ex., or p 13 of [?]).

- 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 [?].

Hartree-Fock-Bogoliubov (HFB) ([?, ?])

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 λN . 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 ρ and a pairing tensor called κ :

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

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

We can make things look *even nicer* if we introduce the following notation representing the mean field Γ and the pairing field Δ :

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

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

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.

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

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

λ_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)

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 [?]

Chapter 2

Time-dependent Hartree-Fock and the inertia tensor

Originally this development is based on [?], 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 [?]

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 ($\mathcal{R} \approx \mathcal{R}_0 \Rightarrow \mathcal{H}_1 \approx 0$)

Chapter 3

RPA vs ATDHF and QRPA vs ATDHFB

I suspect the "Random Phase" in RPA refers to the χ which pops up when we rewrite the density ρ about the HF/HFB ground state density ρ_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 ρ for small perturbations about the ground state, truncating the series at (typically) first- or second-order in χ .

In static RPA, once we've expanded the density and the energy out to second-order in χ , 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 ρ_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 χ again, except this time, χ 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.

Chapter 4

Temperature-dependent Hartree-Fock Bogoliubov

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

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 hairiness¹ to instead describe our system using the grand canonical ensemble, and this turns out to be tractable.

Moving forward by minimizing the grand potential Ω gives us for the density:

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

with associated partition function

¹You 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.

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

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

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

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.

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 of these possible excitations and decided that the number of them was huge (like, 10^{12} huge) [?]. 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 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. The thing that really gets me is that he then does some voodoo black magic to conclude that in FT-DFT, we have to assume that T is constant across the entire PES. That I'm not understanding and I'll have to ask him about that when he gets back.

