TALENT Course: Density functional theory and self-consistent methods

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Lecture 1

Remainder of Quantum Mechanics [Week 1, day 1]

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1.1 The Mathematics of Quantum Mechanics

1.1.1 Vector Space

Quantum mechanics is a theory for the description of the statistical behavior of microscopic entities. It defines physical states in a sesquilinear form of a vector space $\mathcal{H}$ on the field of complex numbers, also known as Hilbert space. **ket** $|a\rangle \in \mathcal{H}$ or **bra** $\langle b| \in \mathcal{H}^*$ (dual space) [1].

Properties of vector spaces:

- addition: $|a\rangle + |b\rangle = |c\rangle$
- scalar product: $\alpha|a\rangle = |a\rangle\alpha$ with $\alpha \in \mathbb{C}$

- inner product: $\langle b|a\rangle = \alpha$ with $\alpha \in \mathbb{C}$
- the inner product is sesquilinear, in other words linear in $|a\rangle$ and anti-linear in $\langle b|$: $\langle b|a + \alpha c\rangle = \langle b|a\rangle + \alpha\langle b|c\rangle$, and $\langle b|a\rangle = \langle a|b\rangle^*$
- and doing so it defines a norm for the vector: $\langle a|a\rangle = ||a||^2 = x \geq 0$, with $x \in \mathbb{R}$

1.1.2 Basis

orthornormal basis $\{|n\rangle\} = \{|1\rangle, |2\rangle, \ldots, |N\rangle\}$ it is an orthonormal basis for the vector space V if $\forall |n\rangle, |m\rangle \in \{|n\rangle\} \Rightarrow |n\rangle \in V$, $\langle n|n\rangle = 1, \langle m|n\rangle = 0$ (normalized and orthogonal), and $\forall |a\rangle \in V \Rightarrow |a\rangle = \sum_{n=1}^{N} c_n|n\rangle$ (complete basis)

1.1.3 Operators

Mathematically operators act on a vector, mapping it from a vector space to another. In Quantum Mechanics operators are **linear** ($(X + \alpha Y)|a\rangle = X|a\rangle + \alpha Y|a\rangle$) and **associative**. In general $X|a\rangle = |b\rangle$, with $|a\rangle \in V$ and $|b\rangle \in W$,

$$X := |b\rangle\langle a|, \tag{1.1}$$

and if we consider a physical state $|a\rangle$ with norm 1

$$X|a\rangle = \langle a|a\rangle|b\rangle = |b\rangle. \tag{1.2}$$

$$\langle m|X|n\rangle := X_{mn} \in \mathbb{C} \tag{1.3}$$

$$X|a\rangle = |b\rangle \Leftrightarrow \langle a|X^\dagger = \langle b|, \text{ with} |b\rangle \in W and \langle b| \in W^*, \tag{1.4}$$

$$(X^\dagger)_{nn'} = X^*_{n'n} \tag{1.5}$$

$$(XY)^\dagger = Y^\dagger X^\dagger \tag{1.6}$$

$X|x\rangle = x|x\rangle$, $x \in \mathbb{C}$ eigenvalue, $|x\rangle \in V$ eigenvector.

Linear operators which satisfy $A^\dagger = A$ are called **Hermitian**, has real eigenvalues.

$$A = \sum_n a_n|n\rangle\langle n|, \qquad a_n \in \mathbb{R} \tag{1.7}$$

Linear operators which satisfy $UU^\dagger = 1 \Rightarrow U^\dagger = U^{-1}$ are called **unitary** ($||Ua||^2 = \langle a|U^\dagger U|a\rangle = ||a||$).

Linear operators which satisfy $P^2 = P$ (idempotency) and are Hermitian, are called orthogonal **projectors**. $P_1|a\rangle = |a_1\rangle \in V_1 \subset V$ and $\langle b|P_1^\dagger(|a\rangle - P_1|a\rangle) = 0$. In the Dirac notation: $P_1 = \sum_{i=1}^{N_1} |i\rangle\langle i|$ where $i = 1 \ldots N_1$ are a subset of the orthonormal basis.

If the case $V_1 \equiv V$, $P_V = \sum_{n=1}^{N} |n\rangle\langle n| \equiv \mathbb{I}$ is the identity operator.

Density operator: $\rho = \sum_i p_i|\psi_i\rangle\langle\psi_i|$, $p_i = |\langle\psi_i|a\rangle|^2$ probability of $|\psi_i\rangle$ in state $|a\rangle$, $|\psi_i\rangle$ is normalized and $\sum_i p_i = 1$

$$\langle A\rangle = \sum_i p_i\langle\psi_i|A|\psi_i\rangle = \mathrm{Tr}[\rho A] \tag{1.8}$$

1.1.4 Tensor Products

$|\phi\rangle_1 = \sum a_n|n\rangle \in \mathcal{H}^{\mathcal{N}}{}_1$, $|_\rangle\chi_2 = \sum c_m|m\rangle \in \mathcal{H}^{\mathcal{M}}{}_2$ Define the tensor products of spaces $|\phi_1 \otimes \chi_2\rangle := |\phi\chi\rangle_{12} = \sum_{n,m} a_n c_m |n \otimes m\rangle_{12} \in \mathcal{H}^{\mathcal{N}}{}_1 \otimes \mathcal{H}^{\mathcal{M}}{}_2$ with dimension $N \cdot M$, is the space of two interacting quantum systems.

$$\langle n \otimes m|n' \otimes m'\rangle_{12} = \delta_{m,m'}\delta_{n,n'}. \tag{1.9}$$

If $A|\phi_1\rangle = a|\phi_1\rangle$,

$$\Rightarrow A|\phi\chi\rangle_{12} = a|\phi\chi\rangle_{12}. \tag{1.10}$$

Two–body Density Matrix

$$\rho_{12} = \rho_1 \otimes \rho_2 = \sum_{i,j} p_i p_j |\phi_i\chi_j\rangle_{12\ 12}\langle\phi_i\chi_j| \tag{1.11}$$

$$\rho_1 = \mathrm{Tr}_2[\rho_{12}] = \sum_m \langle m|\rho_{12}|m\rangle \tag{1.12}$$

1.1.5 Coordinates

An infinite dimensional (with uncountable cardinality) Hilbert space $\mathscr{H}$, is used to represent quantum state that vary in a continuous spectrum, most importantly r and k. The inner product makes use of integrals over wavefunctions and operator which are defined in the sense of the distributions.

Coordinate $|\mathbf{r}\rangle$ and momentum $|\mathbf{k}\rangle$ representations.

$$\hat{\mathbf{r}}|\mathbf{r}\rangle = \mathbf{r}|\mathbf{r}\rangle \tag{1.13}$$

$$\hat{\mathbf{p}}|\mathbf{k}\rangle = \mathbf{k}|\mathbf{k}\rangle \tag{1.14}$$

$$\hat{\mathbf{p}}|\mathbf{r}\rangle = -i\hbar\frac{\mathrm{d}}{\mathrm{d}\mathbf{r}}|\mathbf{r}\rangle \tag{1.15}$$

$$\hat{\mathbf{r}}|\mathbf{k}\rangle = -\frac{1}{i\hbar}\frac{\mathrm{d}}{\mathrm{d}\mathbf{k}}|\mathbf{k}\rangle \tag{1.16}$$

$$\langle\mathbf{r}|\mathbf{k}\rangle = \frac{1}{\sqrt{2\pi\hbar}}e^{\frac{i}{\hbar}\mathbf{r}\cdot\mathbf{k}} \tag{1.17}$$

1.1.6 Variational Principle

Let's consider $|\psi_\lambda\rangle$ eigenvectors of $\hat{H}$, with eigenvalue λ $\hat{H}\,|\psi_\lambda\rangle = \lambda\,|\psi_\lambda\rangle$, forms an orthonormal set $\sum_{\lambda_1,\lambda_2}\langle\psi_{\lambda_1}\mid\psi_{\lambda_2}\rangle = \delta_{\lambda_1\lambda_2}$

Expectation value of h is then given by

$$\langle\psi \mid H \mid \psi\rangle = \sum_{\lambda_1,\lambda_2}\langle\psi|\psi_{\lambda_1}\rangle\,\langle\psi_{\lambda_1}|H|\psi_{\lambda_2}\rangle\,\langle\psi_{\lambda_2}|\psi\rangle \tag{1.18}$$

$$= \sum_\lambda \lambda\,|\langle\psi_\lambda\mid\psi\rangle|^2 \geq \sum_{\lambda\in\mathrm{Spec}(H)} E_0\,|\langle\psi_\lambda\mid\psi\rangle|^2 = E_0 \tag{1.19}$$

so if we minimize E_0 we find the exact expectation value of the Hamiltonian.

1.2 Schroedinger equation

1.2.1 Time dependent and independent Schroedinger Equation

$$\hat{H}\Psi(\mathbf{r},t) = i\hbar\frac{\partial}{\partial t}\Psi(\mathbf{r},t), \tag{1.20}$$

$$\left[\frac{-\hbar^2}{2\mu}\nabla^2 + V(\mathbf{r},t)\right]\Psi(\mathbf{r},t) = i\hbar\frac{\partial}{\partial t}\Psi(\mathbf{r},t). \tag{1.21}$$

If H is time independent than the time evolution and the coordinate evolution are separable.

$$\hat{H}(\mathbf{r})\Psi(\mathbf{r}) = E\Psi(\mathbf{r}), \tag{1.22}$$

with H defined as

$$\left[\frac{-\hbar^2}{2\mu}\nabla^2 + V(\mathbf{r})\right]\Psi(\mathbf{r}) = E\Psi(\mathbf{r}). \tag{1.23}$$

1.2.2 Solutions of time independent Schroedinger equations for notable potentials

1.2.2.1 Free particle Schroedinger equation

One dimensional case $\mathbf{r} \to x$

$V(\mathbf{r}) = 0 \Rightarrow H = T$

$$\hat{H}\psi = E\psi \tag{1.24}$$

$$\frac{-\hbar^2}{2m}\frac{\mathrm{d}}{\mathrm{d}x}\psi(x) = E\psi(x) \tag{1.25}$$

$$\psi(x) = e^{ikx}; \qquad k = \frac{\sqrt{2mE}}{\hbar} \tag{1.26}$$

1.2.2.2 Square well

$$V(x) = \begin{cases} -V_0 & -a/2 < x < a/2 \\ 0 & |x| > a/2 \end{cases} \tag{1.27}$$

if $E < 0$,

$$\psi(x) = A\sin(k_0 x) + B\cos(k_0 x); \qquad k_0 = \frac{\sqrt{2m(E+V_0)}}{\hbar} \qquad |x| < a \qquad -V_0 < E < 0 \tag{1.28}$$

$$\psi(x) = Ce^{kx} + De^{-kx}; \qquad k = -\frac{\sqrt{2m(E)}}{\hbar} \qquad x > a \qquad E < 0 \tag{1.29}$$

$$\psi(x) = Ee^{kx} + Fe^{-kx}; \qquad k = -\frac{\sqrt{2m(E)}}{\hbar} \qquad x < -a \qquad E < 0 \tag{1.30}$$

with $k = \sqrt{2mE}/\hbar$, and $k_0 = \sqrt{2m(E+V_0)}/\hbar$. Since $\psi(x) \in L^2$, $\Rightarrow C = F = 0$ for rinormalizability.

Theorem 1 *If the potential is symmetric, so that $V(x) = V(-x)$, then $\psi(x)$ can be taken as either even or odd.*

for $\psi(x)$ odd $B = 0, D = -F$ $\psi(x) \in C$, so we apply matching conditions for $\psi(x)$ and $\psi'(x)$.

$$k = -\frac{k_0}{\tan(k_0 a)}. \tag{1.31}$$

if $E > 0$, means that also for $|x| > a$ I have positive eigenvalue, so the eigenfunction must be also trigonometric,

$$\psi(x) = A\sin(k_0 x) + B\cos(k_0 x); \qquad k_0 = \frac{\sqrt{2m(E+V_0)}}{\hbar} \qquad |x| < a/2 \qquad -V_0 < E < 0 \tag{1.32}$$

$$\psi(x) = C\sin(kx+\phi) + D\cos(kx+\phi); \qquad k = \frac{\sqrt{2m(E)}}{\hbar} \qquad x > a/2 \qquad E > 0 \tag{1.33}$$

$$\psi(x) = E\sin(kx+\phi) + F\cos(kx+\phi); \qquad k = \frac{\sqrt{2m(E)}}{\hbar} \qquad x > a/2 \qquad E > 0 \tag{1.34}$$

$$\tag{1.35}$$

again I choose to solve the odd case, implying $B = D = F$. Note the phase factor ϕ between the solution inside and outside the well.

using the same technique of matching conditions one obtains,

$$\frac{\mathrm{tg}(ka+\phi)}{k} = \frac{\mathrm{tg}(k_0 a+\phi)}{k_0} \tag{1.36}$$

which has solutions for every k, thus every E defining a continuous energy spectrum. Note that, ϕ is univocally determined,

$$\phi = \mathrm{arctg}\left(\frac{k}{k_0}\mathrm{tg}(k_0 a+\phi)\right) - ka, \tag{1.37}$$

and is related to the *phase shift*.

Moreover considering the matching conditions at $\psi(a)$,

$$\frac{A}{E} = \frac{\sin(ka+\phi)}{\sin(k_0 a)} \tag{1.38}$$

implying that for $\sin(k_0 a) \to 0$, the wavefunction inside the well becomes increasingly important respect to the ones outside defining a resonance for $k_0 a = n\pi$ (Fabry-Perot cavity rule), or $E_n = \frac{(n\hbar\pi)^2}{2ma^2} - V_0$

if I put this square well in a box of length L (or infinite potential well), I have an additional boundary condition that is $\psi(\pm L) = 0$, implying

$$\Rightarrow \sin(ka+\phi) = 0 \Rightarrow E_n = \frac{\hbar^2}{2m}\left(\frac{n\pi}{L} + \phi\right)^2. \tag{1.39}$$

that is not as easy as it seems (remember that ϕ is the solution of a trascendent equation function of k and k_0), but recovers the previous solution for $L >> a$.

1.2.2.3 Harmonic Oscillator

The 1 dimensional harmonic oscillator

$$V = \frac{1}{2} m\omega^2 x^2, \tag{1.40}$$

have solutions with eigenfunctions

$$\psi_n(x) = \frac{1}{\sqrt{2^n\, n!}} \cdot \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} \cdot e^{-\frac{m\omega x^2}{2\hbar}} \cdot H_n\left(\sqrt{\frac{m\omega}{\hbar}} x\right), \tag{1.41}$$

with $H_n(x)$ are Hermite polinomials

$$H_n(z) = (-1)^n\, e^{x^2} \frac{d^n}{dx^n}\left(e^{-x^2}\right), \tag{1.42}$$

and eigenvalues

$$E_n = \hbar\omega\left(n + \frac{1}{2}\right), \tag{1.43}$$

with $n = 0, 1, 2, \ldots$ the *quantum number*.

The three dimensional isotropic harmonic oscillator,

$$V = \frac{1}{2} m\omega^2 r^2 \tag{1.44}$$

is easy to solve considering $r^2 = x^2 + y^2 + z^2$ that gives three independent 1D harmonic oscillators, since the potential is *separable* thus the solution is *factorizable*.

Solving the system in spherical coordinates we use the angular momentum operator $\hat{\mathbf{L}} = \hat{\mathbf{r}} \times \hat{\mathbf{p}}$. A central potential is separable in central and angular part, since

$$\hat{L}^2 |\mathbf{r}\rangle = -\hbar^2 \left[\frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2} + \frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right)\right] |\mathbf{r}\rangle \tag{1.45}$$

that is proportional to angular part of the Laplace operator Δ, corresponding to the operator part of $\hat{\mathbf{p}}^2$, in spherical coordinates.

$$\Rightarrow \hat{\mathbf{p}}^2 = -\hbar^2 \left(\frac{\partial^2}{\partial r^2} + \frac{2}{r}\frac{\partial}{\partial r} \right) + \frac{\hat{L}^2}{r^2} := \hat{p}_r^2 + \frac{\hat{L}^2}{r^2} \tag{1.46}$$

Eigenfunctions of $\hat{L}$ are called spherical harmonics that in spherical coordinates are written as $Y_m^l(\theta, \phi)$. $\hat{L}_z|l,m\rangle = \hbar m|l,m\rangle$ and $\hat{L}^2|l,m\rangle = \hbar^2 l(l+1)|l,m\rangle$. In rotationally invariant systems energy cannot depend from L_i. For a given central interaction,

$$\Rightarrow H = \frac{\hat{p}_r^2}{2m} + \frac{\hat{L}^2}{2mr^2} + V(r) \tag{1.47}$$

we have a system that is separable r and Ω (solid angle), thus its eigensolutions have to be factorized in in eigenfunctions of $\frac{\hat{p}_r^2}{2m} + V(r)$, that we call the *radial part* as $\phi(r)$, and $\frac{\hat{L}^2}{2mr^2}$ that is the *angular part* and are the spherical harmonics.

The solutions for 1.44 are

$$E_{nl} = \hbar\omega \left(2n + l + \frac{3}{2} \right), \tag{1.48}$$

and

$$\phi_{kl}(r) = N_{kl} r^l e^{-\nu r^2} L_k^{(l+\frac{1}{2})}(2\nu r^2), \tag{1.49}$$

with,

$$N_{kl} = \sqrt{\sqrt{\frac{2\nu^3}{\pi}} \frac{2^{k+2l+3}\; k!\; \nu^l}{(2k+2l+1)!!}} \tag{1.50}$$

with $\nu \equiv \frac{\mu\omega}{2\hbar}$ and $L_k{}^{(l+\frac{1}{2})}(2\nu r^2)$ are generalized Laguerre polynomials, that are the solutions to the above differential equation.

Both Hermite and Laguerre polynomials are a orthonormal basis of the Hilbert space, being complete orthogonal basis for L^2. Consequently **spherical harmonics are a basis of the Hilbert space**.

1.3 Spin and Angular momentum

$SO(3)$ is the group of rotations in 3D space, is the group of unitary orthogonal (det= 1) 3x3 matrices. $SU(2)$ is the group of rotations in 2D space, is the group of unitary *special* (det= 1) 2x2 matrices, also known as the Pauli matrices.

$$\sigma_0 = \mathbb{I} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \quad \sigma_1 = \sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_2 = \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_3 = \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{1.51}$$

$\hat{\sigma}$ are the spinor operators for spin 1/2 particles. $\hat{\sigma}, \hat{\mathbf{L}}$, live in different spaces, so $[\hat{\sigma}, \hat{\mathbf{L}}] = 0$. This also means that eigenvectors are factorized $|l,m\rangle \otimes |\pm\rangle$. The two possible state of spins, define a new space called *spinor space*

$$\langle \mathbf{r}|l,m\rangle \otimes |\pm\rangle = \begin{pmatrix} u_{lm}^+(\mathbf{r}) \\ u_{lm}^-(\mathbf{r}) \end{pmatrix} = \begin{pmatrix} \psi^+(\mathbf{r}) \\ \psi^-(\mathbf{r}) \end{pmatrix} Y_m^l(\theta, \phi), \tag{1.52}$$

this representation of wavefunctions in factorized solutions of $\hat{\mathbf{L}}$ and $\hat{\sigma}$, considering a complete set of operators (commute each others) $\hat{L}_z, \hat{\sigma}_z, \hat{\sigma}^2, \hat{L}^2$ is called LS–coupling.

We can define the *total angular momentum*,

$$\hat{\mathbf{J}} := \hat{\sigma} + \hat{\mathbf{L}}, \tag{1.53}$$

we have the following set of complete operators, J^2, L^2, σ^2, J_z, which define the J–coupling scheme. Quantum number $|l - s| \leq j \leq l + s$.

1.4 Exercises

Exercise 1.

demonstrate Eq. (1.5) and (1.6).

Exercise 2.

demonstrate the Schwartz inequality $|\langle a|b\rangle|^2 \leq ||a||^2||b||^2$.

Exercise 3.

exercise: finish problem in Sect. 1.2.2.2, solving the even cases. Then consider the density current

$$\mathbf{j}(\mathbf{r}) = \frac{\hbar}{2im}[\psi(\mathbf{r})\boldsymbol{\nabla}\psi^*(\mathbf{r}) + \psi^*(\mathbf{r})\boldsymbol{\nabla}\psi(\mathbf{r})], \tag{1.54}$$

and calculate how the current density behaves inside and outside the potential well.

Lecture 2

Density functional theory (DFT) [Week 1, day 2]

2.1 Fundamentals of DFT

2-1: Density functional theory I

Density functional theory is based on a constraint variational approach that uses observables as variational parameters.

Let us consider Hamiltonian $\hat{H}$ and observable $\hat{Q}$. Let us assume that the set of parameters $\boldsymbol{p}$ uniquely parametrizes the entire Hilbert space $|\Psi(\boldsymbol{p})\rangle$, that is, $\boldsymbol{p}_1 \neq \boldsymbol{p}_1 \rightarrow |\Psi(\boldsymbol{p}_1)\rangle \neq |\Psi(\boldsymbol{p}_2)\rangle$, and that we can calulate the average values:

$$E(\boldsymbol{p}) = \langle\Psi(\boldsymbol{p})|\hat{H}|\Psi(\boldsymbol{p})\rangle \equiv \langle\hat{H}\rangle, \tag{2.1a}$$
$$Q(\boldsymbol{p}) = \langle\Psi(\boldsymbol{p})|\hat{Q}|\Psi(\boldsymbol{p})\rangle \equiv \langle\hat{Q}\rangle, \tag{2.1b}$$

as well as their derivatives over $\boldsymbol{p}$.

We now solve the constraint variational equation for the routhian $\hat{R}$:

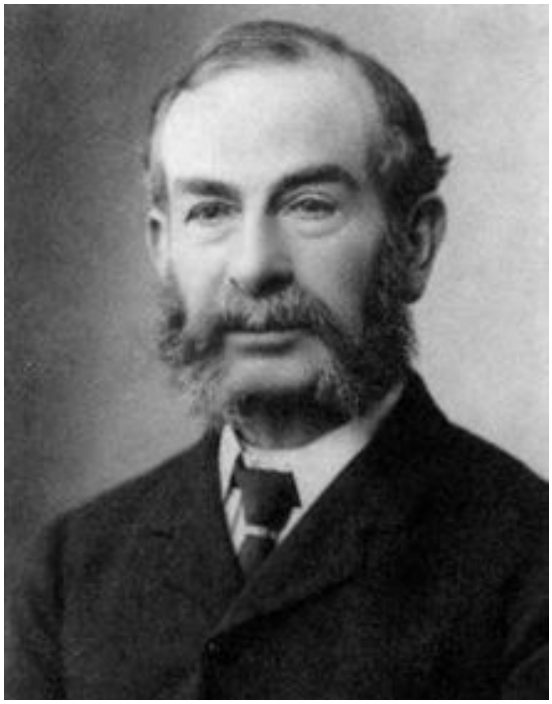
$$\hat{R} = \hat{H} - \lambda\hat{Q}, \tag{2.2}$$

that is,

$$\delta\langle\hat{H}-\lambda\hat{Q}\rangle \equiv \boldsymbol{\nabla}\langle\hat{H}-\lambda\hat{Q}\rangle \equiv \boldsymbol{\nabla}E-\lambda\boldsymbol{\nabla}Q \equiv \frac{\partial}{\partial p_i}\Big[E(\boldsymbol{p})-\lambda Q(\boldsymbol{p})\Big] \equiv \frac{\partial E(\boldsymbol{p})}{\partial p_i}-\lambda\frac{\partial Q(\boldsymbol{p})}{\partial p_i} = 0, \tag{2.3}$$

where λ is called Lagrange multiplier.

2-2: Constraint variation



Edward John Routh FRS; 20 January 1831 – 7 June 1907

Function $E(\boldsymbol{p})$ has a minimum within the set where function $Q(\boldsymbol{p})$ is constant

$$\Updownarrow$$

gradients $\boldsymbol{\nabla} E$ and $\boldsymbol{\nabla} Q$ are parallel.

After solving variational equation (2.3) for all λ we obtain the "path" $\boldsymbol{p}(\lambda)$, and

$$E(\lambda) \equiv E(\boldsymbol{p}(\lambda)), \tag{2.4a}$$
$$Q(\lambda) \equiv Q(\boldsymbol{p}(\lambda)). \tag{2.4b}$$
$$R(\lambda) \equiv R(\boldsymbol{p}(\lambda)) = E(\lambda) - \lambda Q(\lambda). \tag{2.4c}$$

Assuming that function $Q(\lambda)$ can be inverted into $\lambda(Q)$ we obtain

$$E(Q) = \min_{\boldsymbol{p}} E(\boldsymbol{p})\big|_{Q(\boldsymbol{p})=Q} \equiv E(\lambda(Q)) \equiv E(\boldsymbol{p}(\lambda(Q))). \tag{2.5}$$

2-3: Exact ground-state energy E_0 and exact value of observable Q_0

Energy E is now a function of observable Q. By minimizing $E(Q)$, $E_0 = \min_Q E(Q)$ that is, by solving

$$\frac{d}{dQ}E(Q) = 0, \tag{2.6}$$

we obtain E_0 and Q_0

2-4: Density functional theory II

Density functional theory is based on replacing the exact variational method with a two-stage variational method:

1: Minimization of energy E under constraint on value Q of observable $\hat{Q}$, which gives energy $E(Q)$ as function of Q.

2: Minimization of energy $E(Q)$ with respect to Q.

In this way the minimization of energy $E(Q)$ gives the exact ground-state energy E_0 and exact value of observable Q_0.

Depending on which observable we pick, we can have very different DFTs:

$$\delta \left\langle \hat{H} - \lambda \hat{Q} \right\rangle = 0 \implies E = E(Q), \tag{2.7a}$$

$$\delta \left\langle \hat{H} - \sum_{k=1}^{K} \lambda_k \hat{Q}_k \right\rangle = 0 \implies E = E(Q_k), \tag{2.7b}$$

$$\delta \left\langle \hat{H} - \int \mathrm{d}q\, \lambda(q) \hat{Q}(q) \right\rangle = 0 \implies E = E[Q(q)], \tag{2.7c}$$

$$\delta \left\langle \hat{H} + \int \mathrm{d}\boldsymbol{r}\, U(\boldsymbol{r}) \hat{\rho}(\boldsymbol{r}) \right\rangle = 0 \implies E = E[\rho(\boldsymbol{r})], \tag{2.7d}$$

$$\delta \left\langle \hat{H} + \sum_{\sigma} \int \mathrm{d}\boldsymbol{r}\, U(\boldsymbol{r};\sigma) \hat{\rho}(\boldsymbol{r};\sigma) \right\rangle = 0 \implies E = E[\rho(\boldsymbol{r};\sigma)], \tag{2.7e}$$

$$\delta \left\langle \hat{H} + \sum_{\sigma\sigma'} \int \mathrm{d}\boldsymbol{r}\, U(\boldsymbol{r};\sigma'\sigma) \hat{\rho}(\boldsymbol{r};\sigma\sigma') \right\rangle = 0 \implies E = E[\rho(\boldsymbol{r};\sigma\sigma')], \tag{2.7f}$$

$$\delta \left\langle \hat{H} + \sum_{\sigma\tau,\sigma'\tau'} \int \mathrm{d}\boldsymbol{r}\, U(\boldsymbol{r};\sigma'\tau',\sigma\tau) \hat{\rho}(\boldsymbol{r};\sigma\tau,\sigma'\tau') \right\rangle = 0 \implies E = E[\rho(\boldsymbol{r};\sigma\tau,\sigma'\tau')], \tag{2.7g}$$

$$\delta \left\langle \hat{H} + \int \mathrm{d}\boldsymbol{r} \left(U(\boldsymbol{r}) \hat{\rho}(\boldsymbol{r}) + M(\boldsymbol{r}) \hat{\tau}(\boldsymbol{r}) \right) \right\rangle = 0 \implies E = E[\rho(\boldsymbol{r}), \tau(\boldsymbol{r})], \tag{2.7h}$$

$$\delta \left\langle \hat{H} + \int \mathrm{d}\boldsymbol{r} \int \mathrm{d}\boldsymbol{r}\,' U(\boldsymbol{r}\,', \boldsymbol{r}) \hat{\rho}(\boldsymbol{r}, \boldsymbol{r}\,') \right\rangle = 0 \implies E = E[\rho(\boldsymbol{r}, \boldsymbol{r}\,')], \tag{2.7i}$$

$$\delta \left\langle \hat{H} + \int \mathrm{d}x \int \mathrm{d}x'\, U(x', x) \hat{\rho}(x, x') \right\rangle = 0 \implies E = E[\rho(x, x')]. \tag{2.7j}$$

In (2.7j) we denoted $x \equiv \{\boldsymbol{r}, \sigma, \tau\}$ and $x' \equiv \{\boldsymbol{r}', \sigma', \tau'\}$.

Remember that:

2-5: Density functional theory III

> Density functional theory is based on picking the *right observables*, that is, *right degrees of freedom* to describe the given system.

2.1.1 DFT for local densities of spinless particles

Consider DFT (2.7d). One-body density operator is the DFT observable:

$$\hat{\rho}(\boldsymbol{r}) = \sum_{i=1}^{A} \delta(\boldsymbol{r} - \boldsymbol{r}_i) \equiv a^{+}_{\boldsymbol{r}} a_{\boldsymbol{r}}. \tag{2.8}$$

for

$$a_{\boldsymbol{r}} := \sum_{\mu} \phi_{\mu}(\boldsymbol{r}) a_{\mu}, \tag{2.9a}$$

$$a^{+}_{\boldsymbol{r}} := \sum_{\mu} \phi^{*}_{\mu}(\boldsymbol{r}) a^{+}_{\mu}. \tag{2.9b}$$

The position-dependent Lagrange multipliers are identical to one-body (mean-field) potentials $U(\boldsymbol{r})$:

$$\left\langle \hat{U} \right\rangle = \left\langle \int \mathrm{d}\boldsymbol{r}\, U(\boldsymbol{r}) \hat{\rho}(\boldsymbol{r}) \right\rangle = \int \mathrm{d}\boldsymbol{r}\, U(\boldsymbol{r}) \rho(\boldsymbol{r}), \tag{2.10}$$

for

$$\langle \hat{\rho}(\boldsymbol{r}) \rangle = \rho(\boldsymbol{r}). \tag{2.11}$$

The particle-number operator is a sum of density operators:

$$\hat{N} = \int \mathrm{d}\boldsymbol{r}\, \hat{\rho}(\boldsymbol{r}) = \int \mathrm{d}\boldsymbol{r}\, a^{+}_{\boldsymbol{r}} a_{\boldsymbol{r}}, \tag{2.12}$$

This is why:

2-6: Density functional theory IV

Density functional theory based on density observables are universal, that is, applicable to systems of arbitrary particle numbers.

2.1.2 DFT for local densities of spin 1/2 particles

Consider DFT (2.7f).

$$\hat{\rho}(\boldsymbol{r}; \sigma\sigma') = a^{+}_{\boldsymbol{r}\sigma} a_{\boldsymbol{r}\sigma'} \tag{2.13}$$

and

$$\delta = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \quad \sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_x = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \tag{2.14}$$

allows us to introduce scalar and vector (spin) densities and fields:

$$\rho(\boldsymbol{r}; \sigma\sigma') = \tfrac{1}{2}\rho(\boldsymbol{r})\delta_{\sigma\sigma'} + \tfrac{1}{2}\boldsymbol{s}(\boldsymbol{r}) \cdot \boldsymbol{\sigma}_{\sigma\sigma'}, \tag{2.15a}$$

$$U(\boldsymbol{r}; \sigma\sigma') = U(\boldsymbol{r})\delta_{\sigma\sigma'} + \boldsymbol{\Sigma}(\boldsymbol{r}) \cdot \boldsymbol{\sigma}_{\sigma\sigma'}, \tag{2.15b}$$

The interaction energy with the external filed in (2.7f) now reads:

$$\sum_{\sigma\sigma'} \int \mathrm{d}\boldsymbol{r}\, U(\boldsymbol{r}; \sigma'\sigma) \rho(\boldsymbol{r}; \sigma\sigma') = \int \mathrm{d}\boldsymbol{r}\, \left(U(\boldsymbol{r})\rho(\boldsymbol{r}) + \boldsymbol{\Sigma}(\boldsymbol{r}) \cdot \boldsymbol{s}(\boldsymbol{r}) \right), \tag{2.16}$$

and the functional now depends on scalar and vector densities, $E[\rho(\boldsymbol{r}; \sigma\sigma')] = E[\rho(\boldsymbol{r}), \boldsymbol{s}(\boldsymbol{r})]$.

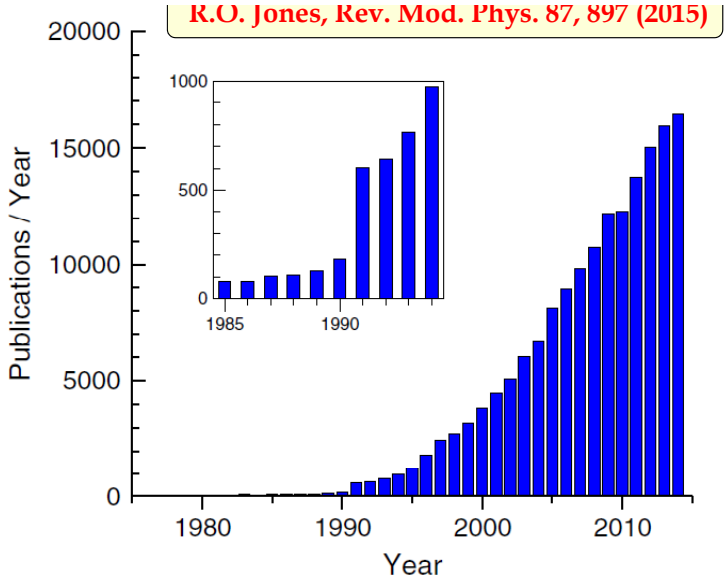


FIG. 1 (color online). Number of publications per year (1975–2014) on topics ("density functional" or "DFT"), according to the Web of Science Core Collection (February 2015). The inset shows data near 1990 on an expanded scale. The number of publications depends on the precise search criteria, but the overall picture is unchanged. From Mavropoulos, 2015.

2.1.3 DFT for local densities of spin 1/2 and isospin 1/2 particles

Consider DFT (2.7g).

$$\hat{\rho}(\boldsymbol{r};\sigma\tau,\sigma'\tau') = a^+_{\boldsymbol{r}\sigma\tau}a_{\boldsymbol{r}\sigma'\tau'} \tag{2.17}$$

and for the isospin density matrices δ and $\boldsymbol{\tau}$,

$$\delta = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \quad \tau_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \tau_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \tau_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \tag{2.18}$$

we introduce scalar and vector, and isoscalar and isovector density matrices [2]:

$$\begin{aligned} \rho(\boldsymbol{r};\sigma\tau,\sigma'\tau') &= \tfrac{1}{4}\rho(\boldsymbol{r})\delta_{\sigma\sigma'}\delta_{\tau\tau'} + \tfrac{1}{4}\boldsymbol{s}(\boldsymbol{r})\cdot\boldsymbol{\sigma}_{\sigma\sigma'}\delta_{\tau\tau'} \\ &+ \tfrac{1}{4}\boldsymbol{\rho}(\boldsymbol{r})\delta_{\sigma\sigma'}\circ\boldsymbol{\tau}_{\tau\tau'} + \tfrac{1}{4}\boldsymbol{s}(\boldsymbol{r})\cdot\boldsymbol{\sigma}_{\sigma\sigma'}\circ\boldsymbol{\tau}_{\tau\tau'}, \qquad (2.19a) \\ U(\boldsymbol{r};\sigma\tau,\sigma'\tau') &= U(\boldsymbol{r})\delta_{\sigma\sigma'}\delta_{\tau\tau'} + \boldsymbol{\Sigma}(\boldsymbol{r})\cdot\boldsymbol{\sigma}_{\sigma\sigma'}\delta_{\tau\tau'} \\ &+ \boldsymbol{U}(\boldsymbol{r})\delta_{\sigma\sigma'}\circ\boldsymbol{\tau}_{\tau\tau'} + \boldsymbol{\Sigma}(\boldsymbol{r})\cdot\boldsymbol{\sigma}_{\sigma\sigma'}\circ\boldsymbol{\tau}_{\tau\tau'}, \qquad (2.19b) \end{aligned}$$

where symbol "$\circ$" denotes the scalar product in the isospace. In another notation we can also write

$$\rho(\boldsymbol{r};\sigma\tau,\sigma'\tau') = \tfrac{1}{4}\sum_{\mu=0}^{3}\sum_{k=0}^{3}\rho_{\mu k}(\boldsymbol{r})\delta^{\mu}_{\sigma\sigma'}\delta^{k}_{\tau\tau'} \tag{2.20a}$$

$$U(\boldsymbol{r};\sigma\tau,\sigma'\tau') = \tfrac{1}{4}\sum_{\mu=0}^{3}\sum_{k=0}^{3}U_{\mu k}(\boldsymbol{r})\delta^{\mu}_{\sigma\sigma'}\delta^{k}_{\tau\tau'} \tag{2.20b}$$

Interaction energy with an external local potential now reads:

$$\begin{aligned}\sum_{\sigma\tau,\sigma'\tau'}\int \mathrm{d}\boldsymbol{r}\, U(\boldsymbol{r};\sigma'\tau',\sigma\tau)\rho(\boldsymbol{r};\sigma\tau,\sigma'\tau') &= \int \mathrm{d}\boldsymbol{r}\Big(U(\boldsymbol{r})\rho(\boldsymbol{r})+\boldsymbol{\Sigma}(\boldsymbol{r})\cdot\boldsymbol{s}(\boldsymbol{r})\\ &\quad +\boldsymbol{U}(\boldsymbol{r})\circ\boldsymbol{\rho}(\boldsymbol{r})+\boldsymbol{\Sigma}(\boldsymbol{r})\cdot\circ\,\boldsymbol{s}(\boldsymbol{r})\Big),\end{aligned} \tag{2.21}$$

and the functional depends on the following densities: scalar-isoscalar $\rho(\boldsymbol{r})$, vector-isoscalar $\boldsymbol{s}(\boldsymbol{r})$, scalar-isovector $\boldsymbol{\rho}(\boldsymbol{r})$, and vector-isovector $\boldsymbol{s}(\boldsymbol{r})$, $E[\rho(\boldsymbol{r};\sigma\tau\sigma'\tau')] = E[\rho(\boldsymbol{r}),\boldsymbol{s}(\boldsymbol{r}),\boldsymbol{\rho}(\boldsymbol{r}),\boldsymbol{s}(\boldsymbol{r})]$.

2.1.4 DFT for quasilocal functional and spinless particles

Consider DFT (2.7i). We first define the operator of local kinetic density $\hat{\tau}(\boldsymbol{r})$ as

$$\hat{\tau}(\boldsymbol{r}) = -\sum_{i=1}^{A}\boldsymbol{\nabla}_i\cdot\delta(\boldsymbol{r}-\boldsymbol{r}_i)\boldsymbol{\nabla}_i \equiv \boldsymbol{\nabla}\Big(a^{+}_{\boldsymbol{r}}\Big)\cdot\boldsymbol{\nabla}\Big(a_{\boldsymbol{r}}\Big), \tag{2.22}$$

for

$$\boldsymbol{\nabla}\Big(a_{\boldsymbol{r}}\Big) := \sum_{\mu}\boldsymbol{\nabla}\Big(\phi_\mu(\boldsymbol{r})\Big)a_\mu, \tag{2.23a}$$

$$\boldsymbol{\nabla}\Big(a^{+}_{\boldsymbol{r}}\Big) := \sum_{\mu}\boldsymbol{\nabla}\Big(\phi^{*}_\mu(\boldsymbol{r})\Big)a^{+}_\mu, \tag{2.23b}$$

and the kinetic density $\tau(\boldsymbol{r})$:

$$\tau(\boldsymbol{r}) = \langle\hat{\tau}(\boldsymbol{r})\rangle = \boldsymbol{\nabla}\cdot\boldsymbol{\nabla}'\rho(\boldsymbol{r},\boldsymbol{r}')\big|_{\boldsymbol{r}'=\boldsymbol{r}}. \tag{2.24}$$

This gives

$$\frac{\hbar^2}{2m}\int \mathrm{d}\boldsymbol{r}\,\hat{\tau}(\boldsymbol{r}) = -\frac{\hbar^2}{2m}\sum_{i=1}^{A}\Delta_i = \hat{T}. \tag{2.25}$$

Densities $\rho(\boldsymbol{r})$ and $\tau(\boldsymbol{r})$ are independent, because for $\boldsymbol{R} = \frac{1}{2}(\boldsymbol{r}+\boldsymbol{r}')$ and $\boldsymbol{s} = \boldsymbol{r}-\boldsymbol{r}'$ we have:

$$\tau(\boldsymbol{R}) = \tfrac{1}{4}\Delta_{\boldsymbol{R}}\rho(\boldsymbol{R},\boldsymbol{s}=0) - \Delta_{\boldsymbol{s}}\rho(\boldsymbol{R},\boldsymbol{s})\big|_{\boldsymbol{s}=0}. \tag{2.26}$$

The first-stage variational equation 2-4 now reads

$$\begin{aligned}&\delta\left\langle\hat{V}+\int\mathrm{d}\boldsymbol{r}\,\left[U(\boldsymbol{r})\hat{\rho}(\boldsymbol{r})+\left(\frac{\hbar^2}{2m}+M(\boldsymbol{r})\right)\hat{\tau}(\boldsymbol{r})\right]\right\rangle\\ &\quad = \delta\left\langle\hat{V}\right\rangle+\delta\int\mathrm{d}\boldsymbol{r}\,\left[U(\boldsymbol{r})\rho(\boldsymbol{r})+\left(\frac{\hbar^2}{2m}+M(\boldsymbol{r})\right)\tau(\boldsymbol{r})\right]=0,\end{aligned} \tag{2.27}$$

which gives the functional:

$$E[\rho,\tau] = \frac{\hbar^2}{2m}\int \mathrm{d}\boldsymbol{r}\,\tau(\boldsymbol{r}) + V[\rho,\tau], \tag{2.28}$$

with the kinetic energy explicitly and exactly singled out.

We now minimize this functional with respect to density and kinetic density under the condition that the number of particles is A. For that we again minimize the Routhian:

$$R[\rho,\tau] = E[\rho,\tau] - \lambda\int \mathrm{d}\boldsymbol{r}\,\rho(\boldsymbol{r}) = \frac{\hbar^2}{2m}\int \mathrm{d}\boldsymbol{r}\,\tau(\boldsymbol{r}) + V[\rho,\tau] - \lambda\int \mathrm{d}\boldsymbol{r}\,\rho(\boldsymbol{r}). \tag{2.29}$$

This gives variational equations:

$$\frac{\delta R[\rho,\tau]}{\delta\rho(\boldsymbol{r})} = \frac{\delta V[\rho,\tau]}{\delta\rho(\boldsymbol{r})} - \lambda = U(\boldsymbol{r}) - \lambda = 0, \tag{2.30a}$$

$$\frac{\delta R[\rho,\tau]}{\delta\tau(\boldsymbol{r})} = \frac{\delta V[\rho,\tau]}{\delta\tau(\boldsymbol{r})} + \frac{\hbar^2}{2m} = M(\boldsymbol{r}) = 0. \tag{2.30b}$$

2-7: Gradient minimization loop

Steepest-descent minimization of the functional $E[\rho,\tau]$ can proceed as follows.

1° Begin with reasonable initial guesses for the densities $\rho^{(0)}(\boldsymbol{r})$ and $\tau^{(0)}(\boldsymbol{r})$. Set the iteration number $k = 0$.

2° Calculate the derivatives:

$$U_{(k)}(\boldsymbol{r}) = \frac{\delta V[\rho^{(k)},\tau^{(k)}]}{\delta\rho^{(k)}(\boldsymbol{r})}, \quad M_{(k)}(\boldsymbol{r}) = \frac{\delta V[\rho^{(k)},\tau^{(k)}]}{\delta\tau^{(k)}(\boldsymbol{r})} + \frac{\hbar^2}{2m}, \tag{2.31}$$

3° Calculate new approximatiosn to densities:

$$\rho^{(k+1)}(\boldsymbol{r}) = \rho^{(k)}(\boldsymbol{r}) - \epsilon(U_{(k)}(\boldsymbol{r}) - \lambda), \tag{2.32a}$$

$$\tau^{(k+1)}(\boldsymbol{r}) = \tau^{(k)}(\boldsymbol{r}) - \epsilon M_{(k)}(\boldsymbol{r}). \tag{2.32b}$$

4° Iterate the loop 2°–3° until convergence is reached.

2.2 Representing densities by orbitals

2-8: N-representability of local density

Arbitrary positive function, $\rho(\boldsymbol{r}) > 0$, normalized as $\int \mathrm{d}\boldsymbol{r}\, \rho(\boldsymbol{r}) = A$, can be represented by a sum of squares of A orthonormal, $\int \mathrm{d}\boldsymbol{r}\, \phi_h^*(\boldsymbol{r})\phi_{h'}(\boldsymbol{r}) = \delta_{hh'}$, functions as

$$\rho(\boldsymbol{r}) = \sum_{h=1}^{A} |\phi_h(\boldsymbol{r})|^2. \tag{2.33}$$

See Refs. [3, 4] and excersise 6 for explicit constructions. The N-representation is, of course, not unique. However, by minimizing the functional with respect to the orbitals, we automatically minimize it with respect to the density. The chain rule rules!

2-9: N-representability of local density and kinetic density?

Conjecture or approximation: Arbitrary positive functions, $\rho(\boldsymbol{r}) > 0$, $\tau(\boldsymbol{r}) > 0$, normalized as $\int \mathrm{d}\boldsymbol{r}\, \rho(\boldsymbol{r}) = A$, can be represented by sums of squares of A orthonormal, $\int \mathrm{d}\boldsymbol{r}\, \phi_h^*(\boldsymbol{r})\phi_{h'}(\boldsymbol{r}) = \delta_{hh'}$, functions as

$$\rho(\boldsymbol{r}) = \sum_{h=1}^{A} |\phi_h(\boldsymbol{r})|^2, \tag{2.34a}$$

$$\tau(\boldsymbol{r}) \simeq \sum_{h=1}^{A} |\boldsymbol{\nabla}\phi_h(\boldsymbol{r})|^2. \tag{2.34b}$$

Generalizations to systems with spin or spin and isospin:

$$\begin{aligned} \langle\Phi|\hat{\rho}(\boldsymbol{r};\sigma\sigma')|\Phi\rangle &= \sum_{h=1}^{A} \phi_h(\boldsymbol{r};\sigma)\phi_h^*(\boldsymbol{r};\sigma') \\ &= \tfrac{1}{2}\rho(\boldsymbol{r})\delta_{\sigma\sigma'} + \tfrac{1}{2}\boldsymbol{s}(\boldsymbol{r})\cdot\boldsymbol{\sigma}_{\sigma\sigma'}, \end{aligned} \tag{2.35a}$$

$$\begin{aligned} \langle\Phi|\hat{\rho}(\boldsymbol{r};\sigma\tau,\sigma'\tau')|\Phi\rangle &= \sum_{h=1}^{A} \phi_h(\boldsymbol{r};\sigma\tau)\phi_h^*(\boldsymbol{r};\sigma'\tau') \\ &= \tfrac{1}{4}\rho(\boldsymbol{r})\delta_{\sigma\sigma'}\delta_{\tau\tau'} + \tfrac{1}{4}\boldsymbol{s}(\boldsymbol{r})\cdot\boldsymbol{\sigma}_{\sigma\sigma'}\delta_{\tau\tau'} \\ &+ \tfrac{1}{4}\boldsymbol{\rho}(\boldsymbol{r})\delta_{\sigma\sigma'}\circ\boldsymbol{\tau}_{\tau\tau'} + \tfrac{1}{4}\boldsymbol{s}(\boldsymbol{r})\cdot\boldsymbol{\sigma}_{\sigma\sigma'}\circ\boldsymbol{\tau}_{\tau\tau'}. \end{aligned} \tag{2.35b}$$

2.3 The DFT Kohn-Sham method

In 1965 Kohn and Sham [5] (Kohn's Nobel Prize 1998) proposed to represent the density by **specific** orbitals.

Let us consider a one-body Kohn-Sham Hamiltonian:

$$\hat{h}_{KS} = -\boldsymbol{\nabla}\left(\frac{\hbar^2}{2m} + M_{KS}(\boldsymbol{r})\right)\cdot\boldsymbol{\nabla} + U_{KS}(\boldsymbol{r}), \tag{2.36}$$

Walter Kohn (March 9, 1923 – April 19, 2016)

where $M_{KS}(\boldsymbol{r})$ and $U_{KS}(\boldsymbol{r})$ are, respectively, the fixed Kohn-Sham mass function and potential. The many-body Kohn-Sham Hamiltonian reads:

$$\hat{H}_{KS} = \sum_{i=1}^{A} \hat{h}_{KS,i} = \int \mathrm{d}\boldsymbol{r} \left[\left(\frac{\hbar^2}{2m} + M_{KS}(\boldsymbol{r}) \right) \hat{\tau}(\boldsymbol{r}) + U_{KS}(\boldsymbol{r}) \hat{\rho}_{KS}(\boldsymbol{r}) \right], \tag{2.37}$$

We know that all eigenstates of a one-body Hamiltonian are equal to Slater determinants $|\Phi_{KS}\rangle$ built of the orbitals diagonalizing $\hat{h}$:

$$\hat{h}_{KS} \phi_h^{KS}(\boldsymbol{r}) = \epsilon_h^{KS} \phi_h^{KS}(\boldsymbol{r}), \tag{2.38}$$

where ϵ_h^{KS} are the Kohn-Sham energies and $\phi_h^{KS}(\boldsymbol{r})$ are the Kohn-Sham orbitals. All average total Kohn-Sham energies, **including the ground-state energy**, read:

$$E_{KS}[\rho_{KS}, \tau_{KS}] = \int \mathrm{d}\boldsymbol{r} \left[\left(\frac{\hbar^2}{2m} + M_{KS}(\boldsymbol{r}) \right) \tau_{KS}(\boldsymbol{r}) + U_{KS}(\boldsymbol{r}) \rho_{KS}(\boldsymbol{r}) \right]. \tag{2.39}$$

for

$$\rho_{KS}(\boldsymbol{r}) = \langle \Phi_{KS} | \hat{\rho}(\boldsymbol{r}) | \Phi_{KS} \rangle = \sum_{h=1}^{A} \phi_h^{KS}(\boldsymbol{r}) \phi_h^{KS*}(\boldsymbol{r}), \tag{2.40a}$$

$$\tau_{KS}(\boldsymbol{r}) = \langle \Phi_{KS} | \hat{\tau}(\boldsymbol{r}) | \Phi_{KS} \rangle = \sum_{h=1}^{A} \left(\boldsymbol{\nabla} \phi_h^{KS}(\boldsymbol{r}) \right) \cdot \left(\boldsymbol{\nabla} \phi_h^{KS*}(\boldsymbol{r}) \right). \tag{2.40b}$$

Are densities $\{\rho_{KS}(\boldsymbol{r}), \tau_{KS}(\boldsymbol{r})\}$ representable by $\{M_{KS}(\boldsymbol{r}), U_{KS}(\boldsymbol{r})\}$? If yes, we can minimize the exact functional $E_{KS}[\rho, \tau]$ in the space of N-representable densities $\{\rho_{KS}(\boldsymbol{r}), \tau_{KS}(\boldsymbol{r})\}$ by using the Kohn-Sham potentials equal to the exact derivatives, that is,

2-10: The Kohn-Sham theorem

Self-consistent minimization of the Kohn-Sham energy E_{KS} with the self-consistency conditions.

$$M_{KS}(\boldsymbol{r}) = \frac{\delta V[\rho, \tau]}{\delta \tau(\boldsymbol{r})}, \quad U_{KS}(\boldsymbol{r}) = \frac{\delta V[\rho, \tau]}{\delta \rho(\boldsymbol{r})}. \tag{2.41}$$

gives the exact solution of the DFT variational equations. The solution is exact up to the approximation of $\tau(\boldsymbol{r}) \simeq \tau_{KS}(\boldsymbol{r})$.

2-11: Self-consistent loop

Self-consistent minimization of the Kohn-Sham energy E_{KS} can proceed as follows.

1° Begin with reasonable initial guesses for the Kohn-Sham potentials $M_{KS}^{(0)}(\boldsymbol{r})$ and $U_{KS}^{(0)}(\boldsymbol{r})$. Set the iteration number $k = 0$.

2° Diagonalize (2.38) the Kohn-Sham hamiltonian $\hat{h}_{KS}^{(k)}$ and find the Kohn-Sham orbitals $\phi_i^{KS,k}(\boldsymbol{r})$.

3° Select A orbitals $\phi_h^{KS,k}(\boldsymbol{r})$, h=1,...,A, from among $i = 1, \ldots, M$ orbitals. Most often the lowest ones.

4° Calculate (2.40) the Kohn-Sham densities $\rho_{KS}^{(k)}(\boldsymbol{r})$ and $\tau_{KS}^{(k)}(\boldsymbol{r})$:

5° Calculate (2.41) the Kohn-Sham potentials $M_{KS}^{(k)}(\boldsymbol{r})$ and $U_{KS}^{(k)}(\boldsymbol{r})$:

6° Iterate the loop 2°–5° until convergence is reached.

2.4 Take-away messages

2.5 Exercises

Exercise 4.

Price of a diver suit depends on the diver's height h and waist w as $E = ah^2 + bw^2$. Within a given population, a company can hire divers of a given stature $Q = ph + qw$. How to minimize

the total cost of buying the diver suits for the company?

$$\frac{\partial R}{\partial h} = 0 \quad \Longrightarrow h = \lambda \frac{p}{2a}, \qquad \frac{\partial R}{\partial w} = 0 \quad \Longrightarrow w = \lambda \frac{q}{2b}. \tag{2.42}$$

$$E(\lambda) = \lambda^2 \left[\frac{p^2}{4a} + \frac{q^2}{4b} \right] \equiv W\lambda^2, \tag{2.43}$$

$$Q(\lambda) = \lambda \left[\frac{p^2}{2a} + \frac{q^2}{2b} \right] \equiv \frac{1}{2} W\lambda, \tag{2.44}$$

$$E(Q) = \frac{4}{W} Q^2, \tag{2.45}$$

$$h_0 = \frac{p}{Wa} Q, \qquad w_0 = \frac{q}{Wb} Q. \tag{2.46}$$

Exercise 5.

Prove the identities

$$\frac{dE(Q)}{dQ} = \lambda, \tag{2.47a}$$

$$\frac{dR(\lambda)}{d\lambda} = Q. \tag{2.47b}$$

Exercise 6.

Prove [4] that any positive function $\rho(y) > 0$ in one dimension, normalized as $\int_0^1 \mathrm{d}y \rho(y) = A$, can be N-represented (2.33) by A orthonormal orbitals as $\rho(y) = \sum_{h=1}^{A} |\phi_h(y)|^2$ for

$$\phi_h(y) = \left[\frac{\rho(y)}{A} \right]^{1/2} \exp\left\{ 2\pi i h \int_0^y \mathrm{d}z \frac{\rho(z)}{A} \right\}. \tag{2.48}$$

Exercise 7.

Using coordinate representation of the kinetic density operator (2.22) prove equations (2.24) and (2.25).

Exercise 8.

Show that equation (2.38) is the variational equation corresponding to minimizing the Kohn-Sham functional (2.39) with respect to the Kohn-Sham orbitals.

Exercise 9.

Derive the Kohn-Sham potentials for the functional (2.28) given by

$$V[\rho,\tau] = \int \mathrm{d}\boldsymbol{r}\, C^{\tau}\rho(\boldsymbol{r})\tau(\boldsymbol{r}) + C^{\rho}\rho^{2}(\boldsymbol{r}) + C_{D}^{\rho}\rho^{2+\alpha}(\boldsymbol{r}), \tag{2.49}$$

where C^{τ}, C^{ρ}, and C_{D}^{ρ} are coupling constants.

$$M(\boldsymbol{r}) = C^{\tau}\rho(\boldsymbol{r}), \quad U(\boldsymbol{r}) = C^{\tau}\tau(\boldsymbol{r}) + 2C^{\rho}\rho(\boldsymbol{r}) + (2+\alpha)C_{D}^{\rho}\rho^{1+\alpha}(\boldsymbol{r}). \tag{2.50}$$

Lecture 3

Second Quantization [Week 1, day 3]

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3.1 The Mathematics of second quantization

We want to describe a relativistic field theory for quantum mechanics. Since in relativity there is no mass conservation, particle number and type is not conserved and has to be defined dinamically. Consequently we will introduce a formalism for many-particle systems called "second quantization"

3.1.1 Fock Space and symmetries

Considering Hilbert space $\mathscr{H}$ of one particle system as defined in sect. 1.1.5 we consider the hilbert space relative to A–particle systems as

$$\mathscr{H}_A = \mathscr{H} \otimes \mathscr{H} \otimes \ldots \otimes \mathscr{H} \tag{3.1}$$

The wavefunctions in this space are $\Phi(x_1, \ldots, x_i, \ldots, x_j, \ldots, x_A)$.

Transposition operator $\hat{P_{ij}}$ which swaps the places of ith and jth particle.

$$\hat{P_{ij}}\Phi(x_1,\ldots,x_i,\ldots,x_j,\ldots,x_A)=\Phi(x_1,\ldots,x_j,\ldots,x_i,\ldots,x_A). \tag{3.2}$$

$\hat{P_{ij}}$ an Hermitian, and unitary operator, so its an operator which eigenvalues can only be $+1$ or -1. We can then divide the space $\mathscr{H}_A$ in space composed of eigenfunctions of $\hat{P_{ij}}$ with eigenvalues $p_{ij}=\pm 1$, $\mathscr{H}_A^{(\pm)}$, and the one orthogonal to these two.

$$\mathscr{H}_A=\mathscr{H}_A^{(+)}\oplus\mathscr{H}_A^{(-)}\oplus\mathscr{H}_A' \tag{3.3}$$

Theorem 2 (Spin Statistic theorem) *Particles living in $\mathscr{H}_A^{(+)}$, with $\hat{P_{ij}}\Phi{=}\Phi$, have integer spin and are called bosons;*
particles living in $\mathscr{H}_A^{(-)}$, with $\hat{P_{ij}}\Phi{=}{-}\Phi$, have semi-integer spin and are called fermions.[6]

$\mathscr{H}_A'$ is the orthogonal complement, populated by functions that are neither symmetric nor anti-symmetric (irreducibile representation of the permutation group), but and up to now is no experimental evidence indicating a connection with physical wavefunctions.

$$\Psi\in\mathscr{H}_2^{(\pm)}\Rightarrow\Phi(x_1\mu,x_2\nu)=\frac{1}{\sqrt{2}}\left(\phi_\mu(x_{P_1})\phi_\nu(x_2)\pm\phi_\mu(x_2)\phi_\nu(x_1)\right) \tag{3.4}$$

When constructing the basis of A-particle states in the space $\mathscr{H}_A^{(-)}$ we similarly single-out **antisymmetric** states,

$$\Phi_{\mu_1\ldots\mu_A}(x_1,\ldots,x_A)=(A!)^{-1/2}\sum_P(-1)^P\phi_{\mu_1}(x_{i_1})\ldots\phi_{\mu_A}(x_{i_A}), \tag{3.5}$$

where P is the permutation of A elements, $\mathrm{P}(1,2\ldots,A){=}(i_1,i_2,\ldots,i_A)$. The above state is called Slater determinant of single-particle states,

$$\Phi_{\mu_1\ldots\mu_A}(x_1,\ldots,x_A)=(A!)^{-1/2}\begin{vmatrix}\phi_{\mu_1}(x_1) & \phi_{\mu_2}(x_1) & \cdots & \phi_{\mu_A}(x_1)\\ \phi_{\mu_1}(x_2) & \phi_{\mu_2}(x_2) & \cdots & \phi_{\mu_A}(x_2)\\ \ldots & \ldots & \ldots & \ldots\\ \phi_{\mu_1}(x_A) & \phi_{\mu_2}(x_A) & \cdots & \phi_{\mu_A}(x_A)\end{vmatrix}. \tag{3.6}$$

Fock space

$$\mathcal{F}^{(\pm)}:=\mathbb{C}\oplus\mathscr{H}\oplus\mathscr{H}_2^{(\pm)}\oplus\cdots\oplus\mathscr{H}_n^{(\pm)}\oplus\cdots \tag{3.7}$$

with functions as

$$f\in\mathcal{F}^{(\pm)}=\begin{pmatrix} f_0 & \in\mathbb{C}\\ f_1(\mathbf{r}_1\sigma_1) & \in\mathscr{H}\\ f_2(\mathbf{r}_1\sigma_1,\mathbf{r}_2\sigma_2) & \in\mathscr{H}_2^{(\pm)}\\ \vdots & \vdots\\ f_n(\mathbf{r}_1\sigma_1,\cdots,\mathbf{r}_n\sigma_n) & \in\mathscr{H}_n^{(\pm)}\\ \vdots & \vdots\end{pmatrix}. \tag{3.8}$$

Applying the number operator results in

$$\hat{N}\Phi = \begin{pmatrix} 0 \cdot f_0 \\ 1 \cdot f_1(\mathbf{r}_1\sigma_1) \\ 2 \cdot f_2(\mathbf{r}_1\sigma_1, \mathbf{r}_2\sigma_2) \\ \vdots \\ n \cdot f_n(\mathbf{r}_1\sigma_1, \cdots, \mathbf{r}_n\sigma_n) \\ \vdots \end{pmatrix}. \tag{3.9}$$

3.1.2 Creation operators

We define a creation operator that creates a particle in the antisymmetric Fock space, thus

$$a_\mu^+ \Phi_A(\mu_1, \cdots, \mu_A) := \begin{cases} 0 & \text{for } \mu \in \{\mu_i\}, \\ \Phi_{A+1}(\mu, \mu_1, \cdots, \mu_A) & \text{for } \mu \notin \{\mu_i\}, \end{cases} \tag{3.10}$$

and the annihilation operator, hermitian conjugate of the constructor, is given by

$$a_\mu \Phi_{A+1}(\mu_1, \cdots, \mu_A + 1) := \begin{cases} 0 & \text{for } \mu \notin \{\mu_i\} \\ (-1)^{i+1} \Phi_A(\mu_1, \cdots, \mu_{i-1}, \mu_{i+1}, \cdots, \mu_{A+1}) & \text{for } \mu = \mu_i \end{cases} \tag{3.11}$$

In $\mathcal{F}^{(-)}$, in other words for fermions, creation and annihilation rules operator obey this following anticommutation rules

$$\left\{a_\mu^+, a_\nu^+\right\} = 0, \tag{3.12}$$

$$\{a_\mu, a_\nu\} = 0, \tag{3.13}$$

$$\left\{a_\mu, a_\nu^+\right\} = \delta_{\mu,\nu}. \tag{3.14}$$

From these relations follows that $a_\mu^+ a_\mu^+ = 0$, that embed the Pauli principle into the properties of the creation operators.

At this point we can define a *vacuum state* such as

$$a_\mu|0\rangle = 0 \qquad \forall\mu \tag{3.15}$$

and every state is defined by application of constructor operators

$$|\mu_1 \cdots \mu_A\rangle := a_{\mu_1}^+ \cdots a_{\mu_A}^+ |0\rangle \tag{3.16}$$

which defines an orthonormal set of states, correspondant to the slater determinant wavefunction in Eq. (3.11).

3.1.3 Operators in second-quantization

$\hat{N}_\nu$ gives the number of fermions occupying the ν-th single-particle state,

$$\hat{N} := \sum_\nu a_\nu^+ a_\nu, \tag{3.17}$$

that is used to define the fermion-number operator:

$$\hat{N}|\mu_1 \ldots \mu_A\rangle = A|\mu_1 \ldots \mu_A\rangle. \tag{3.18}$$

Theorem 3 (Theorem on the second-quantization representation for operators in the Fock space) *In the second-quantization representation, the K-particle operator is defined by its antisymmetrized matrix elements and has the following form:*

$$\hat{F} = (K!)^{-2} \sum_{\substack{\mu_1 \dots \mu_K \\ \nu_1 \dots \nu_K}} F_{\mu_1 \dots \mu_K \nu_1 \dots \nu_K} a^+_{\mu_1} \dots a^+_{\mu_K} a_{\nu_K} \dots a_{\nu_1}, \tag{3.19}$$

that reduces to the case of one and two body operators to

$$\hat{F} = \sum_{\mu_1 \nu_1} F_{\mu_1 \nu_1} a^+_{\mu_1} a_{\nu_1}, \tag{3.20}$$

$$\hat{F} = \frac{1}{4} \sum_{\mu_1 \mu_2 \nu_1 \nu_2} F_{\mu_1 \mu_2 \nu_1 \nu_2} a^+_{\mu_1} a^+_{\mu_2} a_{\nu_2} a_{\nu_1}. \tag{3.21}$$

Creation and destruction operator can also be represented in the Hilbert space (coordinate or momentum), giving the creation or destruction of a particle in a particular position or momentum.

3.1.4 From first to second–quantized form

Let's consider a one body operator in the second quantization form, as in Eq. (3.20), using the field operators as defined in the previous lecture

$$a^+(\mathbf{r}) := \sum_\mu \phi^*_\mu(\mathbf{r}) a^+_\mu, \qquad a(\mathbf{r}) := \sum_\mu \phi_\mu(\mathbf{r}) a_\mu, \tag{3.22}$$

we can build it from first quantization operator

$$\hat{F} = \sum_{\mu_1 \nu_1} \langle \mu | F | \nu \rangle a^+_\mu a_\nu = \int \mathrm{d}^3 r a^+(\mathbf{r}) a(\mathbf{r}) F(\mathbf{r}) \tag{3.23}$$

Implying that densities ($\rho = \sum_i \rho(\mathbf{r} - \mathbf{r}_i)$) in second quantization, at a given coordinate $\mathbf{r}$ are then given by

$$\hat{\rho}(\mathbf{r}) = \hat{a}^+(\mathbf{r}) a(\mathbf{r}) \tag{3.24}$$

3.2 Wick Theorem

Let's consider a decomposition of A on Ψ such as

$$A = A_0 + A_+ + A_-, \tag{3.25}$$

with,

$$A_0 \ \text{ is a constant}, \tag{3.26}$$

$$A_- |\Psi\rangle = 0, \tag{3.27}$$

$$\langle \Psi | A_+ = 0. \tag{3.28}$$

Let then $P{=}|\Psi\rangle\langle\Psi|$ be the operator projecting on the state $|\Psi\rangle$. Thus we get the explicit form of the decomposition (3.25) that fullfills the rules of (3.26-3.28),

$$A_0 = \langle\Psi|A|\Psi\rangle, \tag{3.29}$$

$$A_- = (A - \langle\Psi|A|\Psi\rangle)\,(1-P), \tag{3.30}$$

$$A_+ = (1-P)AP, \tag{3.31}$$

with for any operator A and any state $|\Psi\rangle$.

If we want to calculate the average product of two operators

$$\langle\Psi|AB|\Psi\rangle = \langle\Psi|A|\Psi\rangle\langle\Psi|B|\Psi\rangle + \langle\Psi|A_-B_+|\Psi\rangle, \tag{3.32}$$

that relates to (anti–)commutator relations,

$$\begin{aligned}\langle\Psi|A_-B_+|\Psi\rangle = &\qquad \langle\Psi|\{A_-,B_+\}|\Psi\rangle = \langle\Psi|[A_-,B_+]|\Psi\rangle \\ = &\qquad \langle\Psi|\{A_-,B\}|\Psi\rangle = \langle\Psi|[A_-,B]|\Psi\rangle = \cdots\end{aligned} \tag{3.33}$$

We then define a contraction, and auto–contraction, for fermions as

$$\overbracket{AB} := \{A_-,B\}, \tag{3.34}$$

$$\overbracket{A} := 0. \tag{3.35}$$

To be noted that the contractions for bosons are given by commutator and the auto–contraction is a number that gives an important contribution to observables such as the total energy.

Theorem 4 (Wick's theorem) *If all mutual contractions of pairs of operators in the product are numbers, then the average value of the product of these operators equals the linear combination of products of all possible contractions and auto-contractions.*

$$\overbracket{AD_1D_2\ldots D_kB} := c^k\overbracket{AB}D_1D_2\ldots D_k. \tag{3.36}$$

3.2.1 Wick's theorem for Slater determinants

Owing to anticommutation rules (3.14), fermion contractions are numbers. Can be build considering the configuration which annhilate the state on the left and right (cf. (3.26-3.28)) is called **normal ordering** $N[\cdots]$, and contractions are then defined as

$$\overbracket{AB} = AB - N[AB]. \tag{3.37}$$

They result in the following values,

$$\overbracket{a_\mu^+ a_\nu} = \sum_{i=1}^{A}\delta_{\mu\mu_i}\delta_{\nu\mu_i}, \tag{3.38}$$

$$\overbracket{a_\mu a_\nu^+} = \sum_{i=A+1}^{M}\delta_{\mu\mu_i}\delta_{\nu\mu_i}, \tag{3.39}$$

$$\overbracket{a_\mu^+ a_\nu^+} = \overbracket{a_\mu a_\nu} = 0, \tag{3.40}$$

while auto–contractions vanish:

$$\overset{\sqcap}{a}{}^{+}_{\mu} = \overset{\sqcap}{a}_{\mu} = 0. \tag{3.41}$$

This again is for the specific case of *naked* fermions, we will later see that in the case of other creation and annhilation in other systems contractions and autocontractions can have a different outcome, for example in the system with pairing interaction in the Bolgolybov basis (cf. Lecture 6).

3.2.2 Calculations of matrix elements

Calculation of one body matrix element over two body states gives,

$$\langle \alpha_1', \alpha_2' | \hat{F} | \alpha_1, \alpha_2 \rangle = \sum_{\mu_1 \mu_2 \nu_1 \nu_2} F_{\mu\nu} \langle 0 | a_{\alpha_2'} a_{\alpha_1'} a^+_\mu a_\nu a^+_{\alpha_1} a^+_{\alpha_2} | 0 \rangle \tag{3.42}$$

$$= F_{\alpha_1'\alpha_1}\delta_{\alpha_2'\alpha_2} + F_{\alpha_2'\alpha_2}\delta_{\alpha_1'\alpha_1} - F_{\alpha_1'\alpha_2}\delta_{\alpha_2'\alpha_1} - F_{\alpha_2'\alpha_1}\delta_{\alpha_1'\alpha_2}, \tag{3.43}$$

making use of contractions.

3.3 Exercises

Exercise 10.

Prove that the square of a general one–body operator is equal to a sum of one– and two–body operators.

Exercise 11.

Calculate the matrix elements of a two body operator Eq.(3.21) between two body states using Wick theorem.

Lecture 4

Hartree-Fock Method [Week 1, day 4]

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4.1 Nuclear interaction

The first step to develop a microscopic picture of nuclear structure is to obtain a model for the forces acting between nucleons. The general nuclear Hamiltoninan reads

$$H = \frac{-\hbar^2}{2m}\sum_i \nabla_i^2 + \sum_{i\leq j} v_{ij} + \sum_{i\leq j\leq k} V_{ijk} + \cdots + \text{ n-body terms} \tag{4.1}$$

where v_{ij} is the 2-body Nucleon-Nucleon interaction (NN) and V_{ijk} is the 3-body one.

A possible representation of the 2-body interaction looks like

$$v_{ij} = \sum_{p=1,n} v_p(\mathbf{r}_{ij}) O_{ij}^p \tag{4.2}$$

which is a form factor (typically a sum of Yukawa potential $\sum_a \exp^{-k_a r}/r$) times an operator. To reproduce scattering data a minimum of 8 operators is required

$$O_{ij}^{p=1,8} = 1, \tau_i\tau_j, \sigma_i\sigma_j, (\tau_i\tau_j)(\sigma_i\sigma_j), S_{ij}, S_{ij}(\tau_i\tau_j), \mathbf{L}\cdot\mathbf{S}, \mathbf{L}\cdot\mathbf{S}\tau_i\tau_j \tag{4.3}$$

To reproduce with more accuracy data, extra operators are needed, typically 14 or 18. In Fig.4.1, we show the shape of the NN potential for the different channels of spin and isospin.

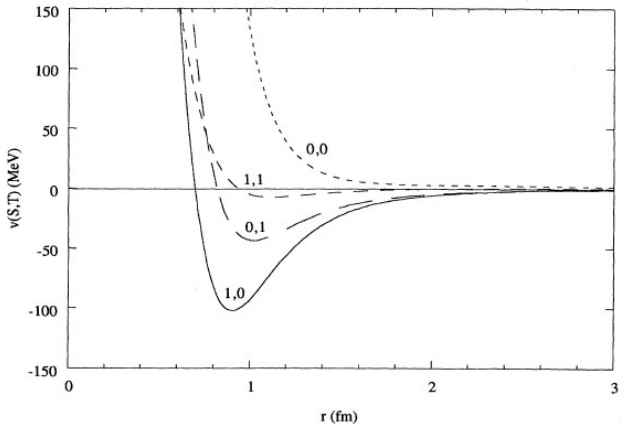

Figure 4.1: Dependence of the Argonne v_{14} NN potential on the total spin (S) and isospin (T). [7].

We observe that the nuclear strong force strongly depends on the spin-isospin channels. It is strongly repulsive at very short distance (hard-core) and attractive at $r \approx 1$ fm. Solving Eq.4.1 for this potential becomes quickly quite prohibitive and thus not applicable to the entire mass chart.

4.1.1 A simple case: Coulomb

The hamiltonian for 1 atom (fixed position) reads (in natural units $\hbar = m_e = \varepsilon_0 = 1$

$$H = -\sum_{i=1}^{n_e} \frac{\nabla_i^2}{2} - Z\sum_{i=1}^{n_e} \frac{1}{r_i} + \sum_{i=1}^{n_e}\sum_{j>i}^{n_e} \frac{1}{r_{ij}} \tag{4.4}$$

We anticipate here that our goal is to find a procedure so that

$$H = \sum_{i=1}^{n_e} h_i^e + \frac{1}{2} \sum_{i=1}^{n_e} \sum_{j>i}^{n_e} \bar{v}^{ee} \tag{4.5}$$

where h_i^e is a single-electron Hamiltonian of the electron i and $\bar{v}^{ee}$ is a residual interaction that is difficult to treat.

4.2 Hartree-Fock method

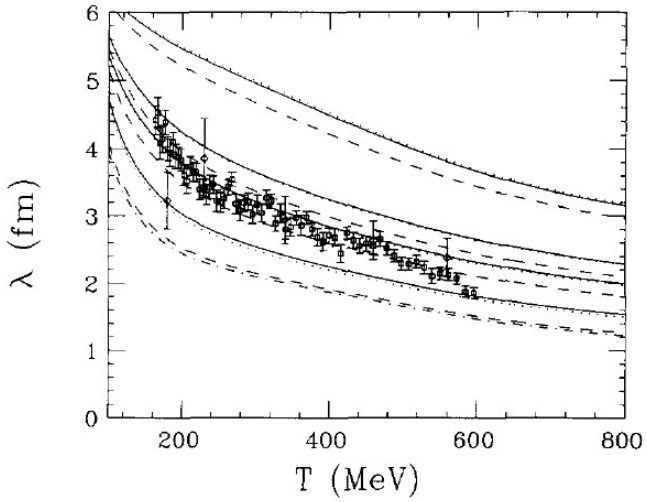

Figure 4.2: Mean free path determined from neutron cross sections (squares) and proton reaction cross sections (diamonds). The solid line represents various theoretical models. [8].

we want to simplify Eq.4.1 by replacing the nuclear potential

$$\sum_{i \leq j} v_{ij} \approx \sum_i v_i \tag{4.6}$$

This means that given a nucleus with A particles. The total Hamiltonian of the system reads now [9]

$$H^{HF} = \sum_i^A h(i) \tag{4.7}$$

The corresponding energy of the system E_0^{HF} can be seen as an approximation to the exact ground state energy of the system. The total wave-function of the system is a *Slater determinant* $\Phi(1, \ldots, A)$

$$|HF\rangle = |\Phi(1,\ldots,A)\rangle = \Pi_i^A a_i^\dagger|-\rangle \tag{4.8}$$

where $a_i^\dagger$ is the single particle creator operator. To calculate the single particle wave functions $\phi_k(i)$ we need to solve a system of coupled equations of the form

$$h(i)\phi_k(i) = \varepsilon_k\phi_k(i) \text{ with } i = (\mathbf{r},\sigma,\tau) \tag{4.9}$$

It is important to recall here that for the Hartree-Fock (HF) case, we replace the initial many-body problem by a simpler one-body problem and. The equation we are going to derive look formally the same as the Kohn-Sham equations of DFT, however there is conceptual difference. While HF is an approximation of the nuclear many-body problem starting from the Hamiltonian, DFT goal is to provide an exact reformulation of the initial problem and can be regarded as an *ab-initio* approach.

4.2.1 Thouless Theorem

The Thouless theorem (Nucl. Phys. 21 1960) states **Theorem**: Any N-particle Slater determinant $|\Phi\rangle$ which is not orthogonal to $|\Phi_0\rangle$ can be written in the form

$$|\Phi\rangle = \Pi_{i=1}^N \Pi_{m=N+1}^\infty (1 + C_{mi}a_m^\dagger a_i)|\Phi_0\rangle \tag{4.10}$$

$$= \exp\left[\sum_{i=1}^N \sum_{m=N+1}^\infty C_{mi}a_m^\dagger a_i\right]|\Phi_0\rangle \tag{4.11}$$

where C_{mi} are uniquely determined.[1]

[1] **proof** We suppose that $\Phi\rangle$ is a determinant of the wave functions

$$\psi_\alpha = \sum_{i=1}^\infty f_{\alpha i}\phi_i \tag{4.12}$$

where $\alpha = 1,\ldots,N$. Using second quantisation we can write the Slater determinant as

$$|\Phi\rangle = \Pi_{\alpha=1}^N \left(\sum_{i=1}^N f_{\alpha i}a_i^\dagger + \sum_{m=N+1}^\infty f_{\alpha m}a_m^\dagger\right)|0\rangle \tag{4.13}$$

Since this state is not orthogonal to $|\Phi_0\rangle$ we have

$$\langle\Phi_0|\Phi\rangle = det f_{\alpha i} = 1 \tag{4.14}$$

here α, i run from 1 to N. We write $F_{i\alpha} = f_{\alpha i}^{-1}$

$$\sum_{i=1}^N f_{\alpha i}F_{i\beta} = \delta_{\alpha\beta} \quad \sum_{\alpha=1}^N F_{i\alpha}f_{\alpha j} = \delta_{ij} \tag{4.15}$$

i,j are less or equal to N. We can thus define $C_{mi} = \sum_{\alpha=1}^N F_{i\alpha}f_{\alpha m}$ for $i \leq N$ and $m > N$. We can now write N linear independent combinations of the wave function $\phi_\alpha$as

The Thouless theorem can be generalised for a more general product state of the form.

Theorem: Each even product state non-orthogonal to vacuum $|0\rangle$ can be uniquely expressed in the following form

$$|\Phi\rangle = Nexp\left\{-\frac{1}{2}\sum_{\mu\nu} Z^{\dagger}_{\mu\nu} a^{\dagger}_{\mu} a^{\dagger}_{\nu}\right\}|0\rangle \tag{4.20}$$

where $Z^T = -Z$ and N is a normalisation constant

4.2.2 Density matrix in Quantum Mechanics

In quantum mechanics, we distinguish between one-particle density matrix, 2-particles, and so on... Formally we can define a single-particle operator in N-body Hilbert space as

$$\hat{\rho}(\mathbf{r}) = \sum_{i=1}^{N} \delta(\mathbf{r} - \hat{\mathbf{r}}_i) \tag{4.21}$$

where $\hat{\mathbf{r}}_i$ is the space operator of particle i and $\mathbf{r}$ is a parameter. We can express it in second quantisation as

$$\hat{\rho}(\mathbf{r}) = \sum_{pq} d_{pq} a^{\dagger}_{p} a_{q} \tag{4.22}$$

$$d_{pq} = \langle p|\delta(\mathbf{r} - \hat{\mathbf{r}})|q\rangle = \sum_{s} \phi^{*}_{p}(\mathbf{r}, s)\phi^{*}_{q}(\mathbf{r}, s) \tag{4.23}$$

The expectation value of this operator on a N-body wave-function is just

---

$$\chi_i = \sum_{\alpha=1}^{N} F_{i\alpha}\psi_{\alpha} = \phi_i + \sum_{m=N+1}^{\infty} C_{mi}\phi_m \tag{4.16}$$

The Slater determinant built out of χ should be equal to $|\Phi\rangle$ so

$$|\Phi\rangle = \left[\Pi_{i=1}^{N} a^{\dagger}_{i} + \sum_{m=N+1}^{\infty} C_{mi} a^{\dagger}_{m}\right]|0\rangle \tag{4.17}$$

$$= \left[\Pi_{i=1}^{N} 1 + \sum_{m=N+1}^{\infty} C_{mi} a^{\dagger}_{m} a_i\right] a^{\dagger}_{i}|0\rangle \tag{4.18}$$

$$= \left[\Pi_{i=1}^{N} \Pi_{m=N+1}^{\infty}(1 + C_{mi} a^{\dagger}_{m} a_i)\right]|\Phi_0\rangle \tag{4.19}$$

The sum over m can be replaced by a product because all terms in which the same creation operator occurs more than one vanish For the same reason we can re-write it in terms of an exponential!.

$$\langle\Psi|\hat{\rho}(\mathbf{r})|\Psi\rangle = N\sum_{spin}\int dr_{2,...N}|\Psi(\mathbf{r},s,\mathbf{r}_2,s_2,....\mathbf{r}_N,s_N)|^2 = \rho(\mathbf{r}) \tag{4.24}$$

this can be interpreted as the diagonal element of an operator $\hat{\rho}_\Psi$ in coordinate space and called *density matrix*.

$$\langle\mathbf{r}s|\hat{\rho}_\Psi|\mathbf{r}'s'\rangle = \rho(\mathbf{r}s\mathbf{r}'s') = \sum_{pq}\phi_p(\mathbf{r}.s)\rho_{qp}\phi_q^*(\mathbf{r}'s') \tag{4.25}$$

with $\rho_{qp} = \langle\Psi|c_q^\dagger c_p|\Psi\rangle$ being the matrix element of the density operator in arbitrary basis.

For the specific case of a Slater determinant, ρ is diagonal in a given single-particle basis $\hat{\rho}_\Psi^2 = \hat{\rho}_\Psi$

We can consider elements of a density matrix as measurable characteristics of a product state. For example, measuring a physical quantity, which corresponds to a one-body or two-body operator, on a product state, we respectively obtain

$$\langle\Phi|\hat{F}|\Phi\rangle = \sum_{\mu\nu}F_{\mu\nu}\rho_{\nu\mu} = TrF\rho \tag{4.26}$$

$$\langle\Phi|\hat{F}|\Phi\rangle = \frac{1}{2}\sum_{\mu\mu'\nu\nu'}F_{\mu\mu'\nu\nu'}\rho_{\nu\mu}\rho_{\nu'\mu'} \tag{4.27}$$

4.2.3 Deriving HF equations

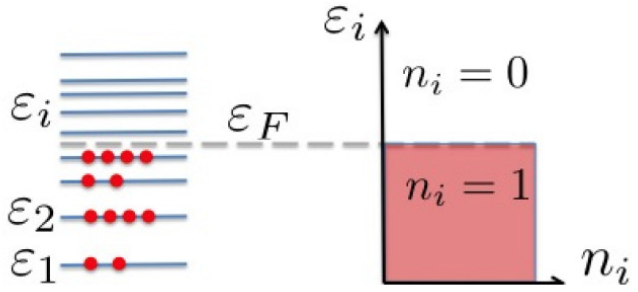

Figure 4.3: Single particle leveles and occupation probability of the states. ε_F is the Fermi energy, defined as the energy between the last occupied and first empty state.

To derive HF equation we use Thouless theorem to build a class of trial functions of a A system We introduce the notation $p = A+1,...M$ (particle) and $h = 1,..,A$ (hole)

$$|\tilde{Z}\rangle = \exp(\sum_{ph}Z_{ph}^* a_p^\dagger a_h)a_1^\dagger...a_A^\dagger|0\rangle \tag{4.28}$$

Z_{ph} is a rectangular matrix.

We define the HF energy as

$$E_{HF} = \frac{\langle \tilde{Z}|H|\tilde{Z}\rangle}{\langle \tilde{Z}|\tilde{Z}\rangle} \tag{4.29}$$

The variational principle $\delta E_{HF} = 0$ means

$$\delta E_{HF} = \frac{\langle \tilde{Z}|H|\delta_\perp \tilde{Z}\rangle}{\langle \tilde{Z}|\tilde{Z}\rangle} \tag{4.30}$$

notice we have performed a orthogonal variation of $|\tilde{Z}\rangle$

$$|\delta_\perp \tilde{Z}\rangle = |\delta \tilde{Z}\rangle - \frac{\langle \tilde{Z}|\delta \tilde{Z}\rangle}{\langle \tilde{Z}|\tilde{Z}\rangle}|\tilde{Z}\rangle \tag{4.31}$$

We define

$$\delta := \sum_{ph} \delta Z^*_{ph} \frac{\partial}{\partial Z^*_{ph}} \tag{4.32}$$

We have

$$|\delta \tilde{Z}\rangle = \sum_{ph} \delta Z^*_{ph} a^\dagger_p a_h |\tilde{Z}\rangle \tag{4.33}$$

$$|\delta_\perp \tilde{Z}\rangle = \sum_{ph} \delta Z^*_{ph} \left(a^\dagger_p a_h - \rho_{hp}\right)|\tilde{Z}\rangle \tag{4.34}$$

$$\tag{4.35}$$

We get

$$\delta E_{HF} = \frac{\langle \tilde{Z}|H|\delta_\perp \tilde{Z}\rangle}{\langle \tilde{Z}|\tilde{Z}\rangle} \tag{4.36}$$

$$= \frac{1}{\langle \tilde{Z}|\tilde{Z}\rangle}\langle \tilde{Z}|H|\sum_{ph} \delta Z^*_{ph} \left(a^\dagger_p a_h - \rho_{hp}\right)|\tilde{Z}\rangle \tag{4.37}$$

that we have to put to zero thus

$$\langle \tilde{Z}_0|H|\left(a_p^\dagger a_h - \rho_{0hp}\right)|\tilde{Z}_0\rangle = 0 \tag{4.38}$$

where "0" means a product state that obeys this variational principle.

Apply Wick on the Hamiltonian

$$H = T + V = \sum_{\mu\nu} T_{\mu\nu} a_\mu^\dagger a_\nu + \frac{1}{4}\sum_{\mu\lambda\nu\pi} V_{\mu\lambda\nu\pi} a_\mu^\dagger a_\lambda^\dagger a_\pi a_\nu \tag{4.39}$$

by doing that we get

$$\begin{aligned} \langle \tilde{Z}|H|\left(a_\mu^\dagger a_\nu - \rho_{\nu\mu}\right)|\tilde{Z}\rangle &= \langle \tilde{Z}|H|a_\mu^\dagger a_\nu|\tilde{Z}\rangle - \rho_{\nu\mu}\langle \tilde{Z}|H|\tilde{Z}\rangle & (4.40)\\ &= (\rho h(1-\rho))_{\mu\nu} & (4.41)\end{aligned}$$

where $h_{\mu\nu} = T_{\mu\nu} + \Gamma_{\mu\nu}$. T is the one-body matrix elements of the kinetic term and $\Gamma_{\mu\nu} = \sum_{\lambda\pi} V_{\mu\lambda\nu\pi}\rho_{\pi\lambda}$. From the hermiticity of the interaction we conclude that

$$\Gamma^\dagger = \Gamma \tag{4.42}$$
$$h^\dagger = h \tag{4.43}$$

We can summarise the result by showing that the product state $|\tilde{Z}_0\rangle$ obeys the variational Hartree-Fock condition if its density matrix ρ_0 obeys

$$[h_0, \rho_0] = 0 \tag{4.44}$$

The density matrix obeying the Hartree-Fock equation is called self-consistent density matrix and the Hamiltonian induced by it - self-consistent Hamiltonian

To solve this equation we have to set up a self-consistent procedure as illustrated in Fig.4.4

We can now calculate the HF energy

$$\begin{aligned} E^{HF} &= TrT\rho + \frac{1}{2}TrTr(\rho\bar{v}\rho) & (4.45)\\ &= TrT\rho + \frac{1}{2}Tr(\rho\Gamma) & (4.46)\\ &= TrT\rho + \frac{1}{2}Tr(\rho h - \rho T) & (4.47)\\ &= \frac{1}{2}TrT\rho + \frac{1}{2}Trh\rho & (4.48)\end{aligned}$$

in canonical basis

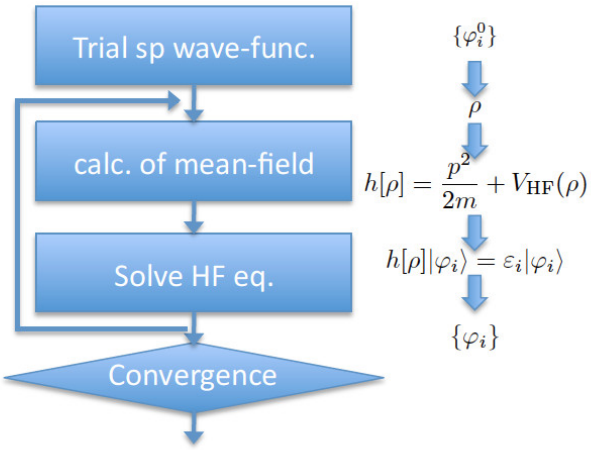

Figure 4.4: Self-consistent procedure used to solve HF equations. First one has to choose a set of single-particle states that are supposed to not be too far from the solution.Then, from them, the HF hamiltonian is computed. Bysolving HF equations, new single-particle states are found. Then, the procedure is iterated until the convergence is achieved

$$E^{HF} = \frac{1}{2}\sum_{h=1}^{A}(T_{hh} + \varepsilon_h) \tag{4.49}$$

T_{hh} are the diagonal matrix element of the kinetic energy operator

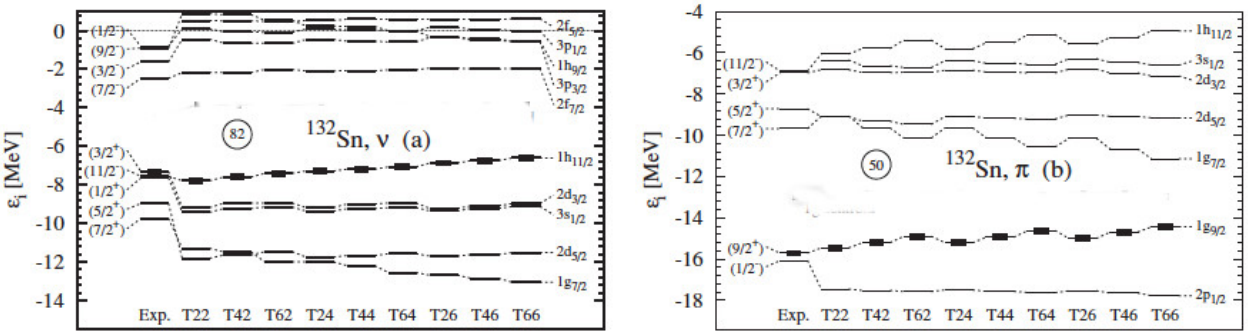

Figure 4.5: Single particle energies in ^{132}Sn for some given interactions (Skyrme family) for neutron states (a) and protons (b). A thick mark indicates the Fermi level. Taken from Ref. [10].

Single particle states are not strictly speaking observables, but they can be associated with the necessary energies to add/remove a particle from a N-body system. In particular we make use of the so called Koopman's theorem

$$E^{HF}[N+1] - E^{HF}[N] \approx \varepsilon_{N+1} \tag{4.50}$$

which states that the energy difference between to nuclei with N and N+1 particles corresponds to the single particle energy ε_{N+1} of the last occupied state.

4.2.4 Stability matrix

We derived the Hartree-Fock equations requiring that the first variation of energy equal zero To see if the solution corresponds to a real minimum of the total energy we have to consider the second order variation of the energy.

Let assume that the density matrix ρ can be expanded around ρ_0

$$\begin{aligned} \rho &= \rho_0 + \rho_1 + \rho_2 + \dots && (4.51) \\ \rho_0 &\geq \rho_1 \geq \rho_2 \dots && (4.52) \end{aligned}$$

by requiring that the ρ matrix is a projector, we have

$$\begin{aligned} \rho_0^2 &= \rho_0 && (4.53) \\ \rho_0\rho_1 + \rho_1\rho_0 &= \rho_1 && (4.54) \\ \rho_0\rho_2 + \rho_1\rho_1 + \rho_2\rho_0 &= \rho_2 && (4.55) \end{aligned}$$

We define $\sigma_0 = 1 - \rho_0$, which is still a projector. We consider an arbitrary matrix A.

$$\begin{aligned} \rho_0[A,\rho_0]\rho_0 = \sigma_0[A,\rho_0]\sigma_0 = 0 && (4.56) \\ \rho_0[A,\rho_0]\sigma_0 = -\rho_0 A\sigma_0 && (4.57) \\ \sigma_0[A,\rho_0]\rho_0 = \sigma_0 A\rho_0 && (4.58) \end{aligned}$$

since ρ_0 projects on occupied (hole) states and σ_0 on unoccupied (particle) states, we can separate A in blocks $h = 1, A$ $p = A+1, \dots, M$

$$[A,\rho_0] = \begin{pmatrix} 0 & -A_{hp} \\ A_{ph'} & 0 \end{pmatrix} \quad (4.59)$$

$$[[A,\rho_0],\rho_0] = \begin{pmatrix} 0 & -A_{hp} \\ A_{ph'} & 0 \end{pmatrix} \quad (4.60)$$

$$(4.61)$$

If we now come back to Eq.4.56, we can re-write them as

$$\rho_1 = [[\rho_1, \rho_0], \rho_0] \tag{4.62}$$

$$\rho_2 = [[\rho_2, \rho_0], \rho_0] + \frac{1}{2}[[\rho_1, \rho_0], \rho_1] \tag{4.63}$$

this means that the pp and hh matrix elements of first order correction ρ_1 are equal to zero, while the same matrix elements of ρ_2 depended on the correction ρ_1.

Since we have ρ_0 the HF density we need to discuss only second order variation E_2. We defined the stability operator of the solution of HF equations, which acts in the set of Hermitian matrices with vanishing p-p and h-h elements as a linear transformation is defined as

$$M_0\rho_1 := [[h_0, \rho_1] + [\Gamma_1, \rho_0], \rho_0] \tag{4.64}$$

We see that the second order energy variation around the HF solution depends only on the first-order variation of the density matrix.

Theorem Second-order variation of energy around the HF solution is equal to the diagonal matrix element of the Hermitian stability operator M_0 calculated for first-order correction to the density

$$E_2 = \frac{1}{2}(\rho_1|M_0\rho_1) \tag{4.65}$$

We have used the scalar product of 2 matrices as $(A|B) = TrA^\dagger B$. In the canonical basis of HF density the stability matrix reads

$$(M_0\rho_1)_{ph} = (e_p - e_h)\rho_{1ph} + \sum_{p'h'}(V_{pp'hh'}\rho_{1h'p'} + V_{ph'hp'}\rho_{1p'h'}) \tag{4.66}$$

we will see that this matrix is related to RPA equations. To get a stable HF solution we need to have such a matrix to be positive definite, this check can be done only numerically..

4.3 Infinite nuclear matter

As a first example of applications of HF to a system, we consider the infinite medium.

$$\phi_{\mathbf{k}}(\mathbf{r}) = \frac{1}{\sqrt{\Omega}}\exp^{-i\mathbf{kr}}\chi_{\frac{1}{2}\sigma}\chi_{\frac{1}{2}\tau} \tag{4.67}$$

The infinite medium is characterized by the density

$$\rho_0 = \rho_{n\uparrow} + \rho_{p\uparrow} + \rho_{n\downarrow} + \rho_{p\downarrow} \tag{4.68}$$

We can thus characterise the infinite medium by considering the unbalance between the different densities. In the following we will consider only spin-saturated system ($\rho_\uparrow = \rho_\downarrow$), but it it simple to generalise. We define an asymmetry parameter

$$Y = \frac{\rho_n - \rho_p}{\rho_n + \rho_p} \tag{4.69}$$

we have thus the two important cases $Y = 0$ Symmetric Nuclear Matter (SNM) and Y=1 Pure Neutron Matter.

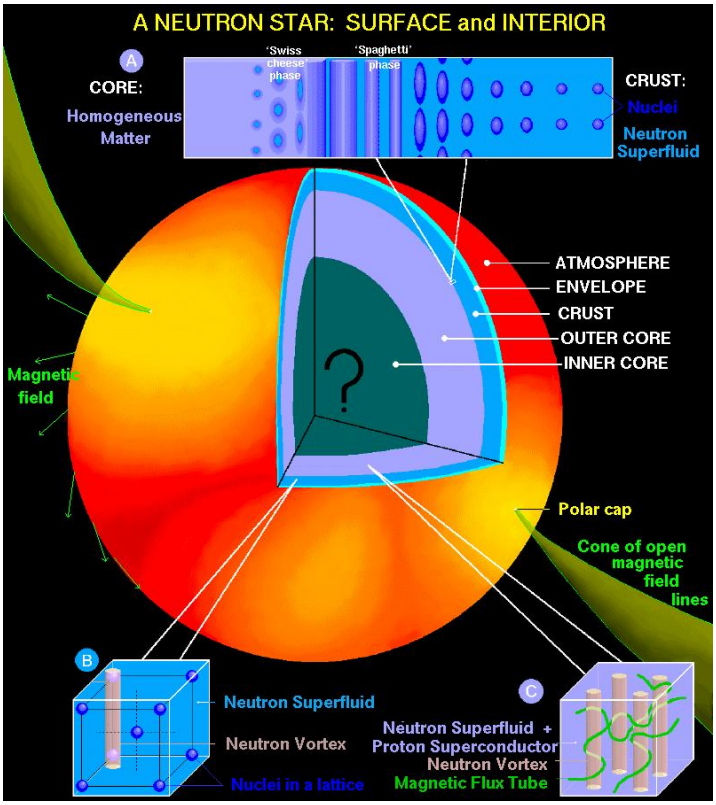

Figure 4.6: Schematic representation of a Neutron Star

The HF Hamiltonian is composed by a kinetic part (treated as Fermi gas) and interaction. We consider SNM (thus $\rho_n = \rho_p$)

The expectation value of the kinetic energy is

$$\left.\frac{E}{A}\right|_{Kinetic} = \frac{3}{5}\frac{\hbar^2}{2m}k_F^2 \tag{4.70}$$

Exercise 4 Prove the previous result on kinetic energy. Assume at first no interaction and a pure Fermi gas. Remember that $\sum_{\mathbf{k}} \to \frac{1}{(2\pi)^3}\int d^3k$ *and* $k_F^3 = \frac{3}{2}\pi^2\rho$

While for the the interaction V one needs to calculate explicitly

$$\langle V\rangle = \frac{1}{2}\sum_{i,j\leq\varepsilon_F}\langle i,j|V(r)(1-P_\sigma P_\tau P_x)|ij\rangle \tag{4.71}$$

the exchange operator $P_\sigma P_\tau P_x$ acting on spin/isospin/position gives us the Fock term. Let's make explictly the calculation taking an interaction of the form

4.3.1 Example: finite range interactions

$$V(r) = W\exp^{-(r_1-r_2)^2/\mu^2} \tag{4.72}$$

Recalling that momentum and spin commute we can calculate the following quantities

$$4P_\sigma P_\tau = 1-\sigma_1\sigma_2-\tau_1\tau_2+\sigma_1\sigma_2\tau_1\tau_2 \tag{4.73}$$

We have

$$\begin{aligned}
\langle V\rangle_{SNM} &= \frac{1}{2}W\sum_{ij}\langle ij|V(r)(1-P_\sigma P_\tau P_x)|ij\rangle \\
&= \frac{1}{2}4\times 4\sum_{k_ik_j}\langle k_ik_j|W\exp^{-(r_1-r_2)^2/\mu^2}\left(1-\frac{1}{4}P_x\right)|k_ik_j\rangle \\
&= 8\sum_{k_ik_j}\frac{1}{\Omega^2}\int d^3r_1d^3r_2W\exp^{-(r_1-r_2)^2/\mu^2}\left[1-\frac{1}{4}\exp^{-i(\mathbf{k}_i-\mathbf{k}_j)(\mathbf{r}_1-\mathbf{r}_2)}\right] \\
&\quad [\text{From } r_1,r_2 \text{ to center of mass coordinates so we can get rid on 1 integral } R, r_{12}] \\
&= \frac{8}{\Omega}\sum_{k_ik_j}\int d^3r_{12}W\exp^{-(r_1-r_2)^2/\mu^2}\left[1-\frac{1}{4}\exp^{-i(\mathbf{k}_i-\mathbf{k}_j)\mathbf{r}_1}\right] \\
&= \frac{8}{\Omega}\left(\frac{\Omega}{8\pi^3}\right)^2\int d^3k_id^3k_j\int d^3r_{12}W\exp^{-(r_1-r_2)^2/\mu^2}\left[1-\frac{1}{4}\exp^{-i(\mathbf{k}_i-\mathbf{k}_j)\mathbf{r}_1}\right]
\end{aligned} \tag{4.74}$$

We now define

$$\mathcal{V}(0) = \int d^3r\exp^{-(r_1-r_2)^2/\mu^2} \tag{4.75}$$

$$\mathcal{V}(k) = \int d^3r\exp^{i\mathbf{kr}}\exp^{-(r_1-r_2)^2/\mu^2} \tag{4.76}$$

and we have

$$\langle V\rangle_{SNM} = W\frac{\Omega}{8\pi^6}\left\{\left(\frac{4\pi}{3}k_F^3\right)^2\mathcal{V}(0) - \frac{1}{4}\int d^3k_i d^3k_j \mathcal{V}(k)\right\} \tag{4.77}$$

Notice that the integral over the two Fermi spheres is limited by the HF to the two Fermi momenta k_{F1}, k_{F2} which are equal in this case.

$$\frac{1}{A}\langle V\rangle = \frac{1}{2}\rho W\left\{\prime - 3\int_0^1 dx x^2(2+x^3-3x)(2k_F x)\right\} \tag{4.78}$$

$$E = a_V A - a_s A^{2/3} - a_C Z^2/A^{1/3} - a_A(A-2Z)^2/A + \ldots \tag{4.79}$$

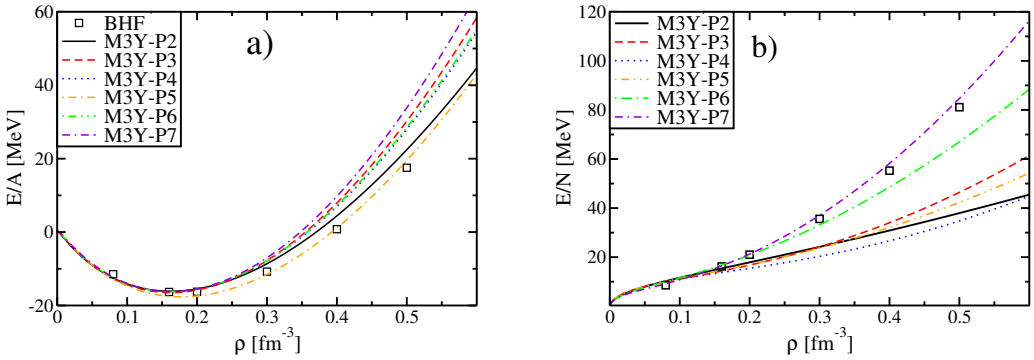

Figure 4.7: Energy per particle in SNM (panel a) and PNM (panle b) for some effective interactions at HF level. symbols refer to ab-initio results based on BHF.

4.3.2 Example: zero range interactions

Consider an interaction of the type

$$V = t_0(1+x_0P_\sigma)\delta(r_i-r_j) + \frac{1}{6}t_3(1+x_3P_\sigma)\rho\left(\frac{r_i+r_j}{2}\right)^\alpha\delta(r_i-r_j) \tag{4.80}$$

this is the simplest form of the Skyrme interaction.

$$\begin{aligned}(1+x_0P_\sigma)(1-P_xP_\sigma P_\tau) &= (1+x_0P_\sigma)(1-P_\sigma P_\tau) &(4.81)\\ &= 1+x_0P_\sigma-(x_0P_\sigma^2+P_\sigma)P_\tau &(4.82)\\ &= 1+\frac{1}{2}x_0-\frac{1}{2}(1+2x_0)P_\tau &(4.83)\end{aligned}$$

where $P_x = 1$ is due to the fact that the δ is a pure S-wave. We have

$$\begin{aligned} E_{HF} &= \frac{t_0}{2}\sum_{lm}\int \psi_l^*(r_i')\psi_m^*(r_j')\left(1+\frac{1}{2}x_0-\frac{1}{2}(1+2x_0)P_\tau\right)\psi_l(r_i)\psi_m(r_j)dr_i dr_j dr_{i'}dr_{j'}\big|_{r_i=r_j=r_i'=r_j'} \\ &= \int\left\{\frac{t_0}{2}\left(1+\frac{1}{2}x_0\right)\rho(r_i,r_i')\rho(r_i,r_i')-\frac{t_0}{2}(\frac{1}{2}+x_0)\rho(r_i,r_i')\rho(r_i,r_i')\delta_{q_1q_2}\right\}dr_i dr_j dr_{i'}dr_{j'}\big|_{r_i=r_j=r_i'=r_j'} \\ &= \int d^3r\left\{\frac{t_0}{2}\left(1+\frac{1}{2}x_0\right)\rho(r)^2-\frac{t_0}{2}(\frac{1}{2}+x_0)\sum_q\rho_q(r)^2\right\} \end{aligned} \tag{4.84}$$

where P_τ reduces to a $\delta_{q_1q_2}$ since we assume no isospin mixing. For SNM we have (leave as exercise)

$$\left.\frac{E}{A}\right|_{SNM} = \frac{3t_0}{8}\rho+\frac{t_3}{16}\rho^{\alpha+1} \tag{4.85}$$

From the simple HF calculation of the infinite medium we can extract extra informations on the nuclear interaction

$$P = \rho^2\frac{\partial E/\rho}{\partial\rho} \text{ [pressure]} \tag{4.86}$$

$$K = 9\frac{\partial P}{\partial\rho} \text{ [incompressibility]} \tag{4.87}$$

$$E/A(\rho,Y) = E/A(\rho,0)+S(\rho)Y^2+\ldots \text{ [symmetry energy]} \tag{4.88}$$

$$L = 3\rho\frac{\partial S}{\partial\rho} \text{ [slope of symmetry energy]} \tag{4.89}$$

These quantities can be related to properties of finite nuclei as neutron skin-thickness (L) or the centroid of giant monopole resonances. See Figs.4.8-4.9

4.3.3 Neutron Stars

To calculate the mass and the radius of a NS we have to solve the Tolman-Oppenheimer-Volkoff (TOV) equations for the total pressure P and the enclosed mass m

$$\begin{aligned} \frac{dP(r)}{dr} &= -\frac{Gm(r)\varepsilon(r)}{r^2}\left[\left(1+\frac{P(r)\varepsilon(r)}{c^2}\right)\left(1+\frac{4\pi r^3P(r)}{\varepsilon(r)c^2}\right)\right]\left[1-\frac{2Gm(r)}{rc^2}\right]^{-1}, \\ \frac{dm(r)}{dr} &= 4\pi r^2\varepsilon(r)\,, \end{aligned} \tag{4.90}$$

where G is the gravitational constant and $\varepsilon(r)$ is the total energy density of the system [We need to include mass contribution!!].

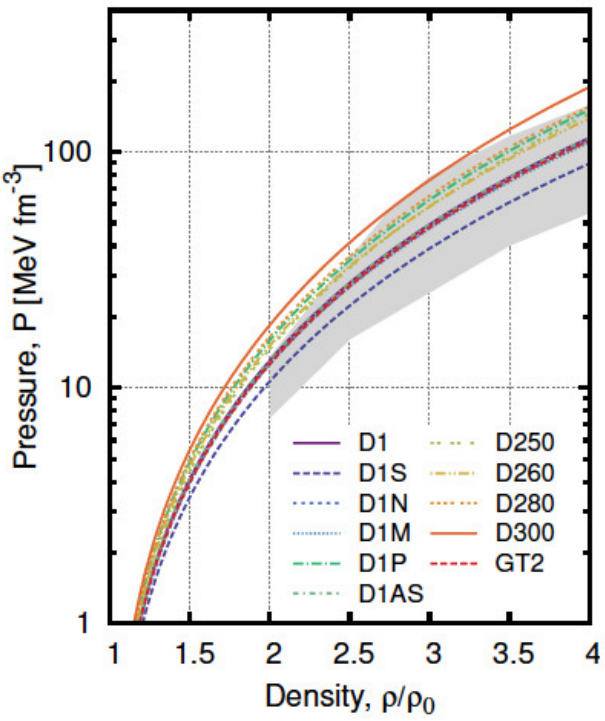

Figure 4.8: Evolution of pressure in SNM for different interaction (Gogny). The shaded area is a constraint extracted from flow data experiment Ref. [11]. Taken from Ref. [12]

4.4 Exercise

Exercise 11

Given the simple equation of state

$$\left.\frac{E}{A}\right|_{SNM} = \frac{3t_0}{8}\rho + \frac{t_3}{16}\rho^{\alpha+1} \tag{4.91}$$

Find a set of values t_0, t_3 that gives you a *reasonable* equation of state:

$$\left.\frac{E}{A}\right|_{\rho=\rho_{sat}} \approx -16MeV$$
$$\rho_{sat} \approx 0.16fm^{-3}$$

The parameter α is usually take in the region $\alpha \in [0.1 - 1]$. A good EoS should not collapse at large densities $i.e. \frac{E}{A} > 0$ for $\rho > 3 \times \rho_{sat}$

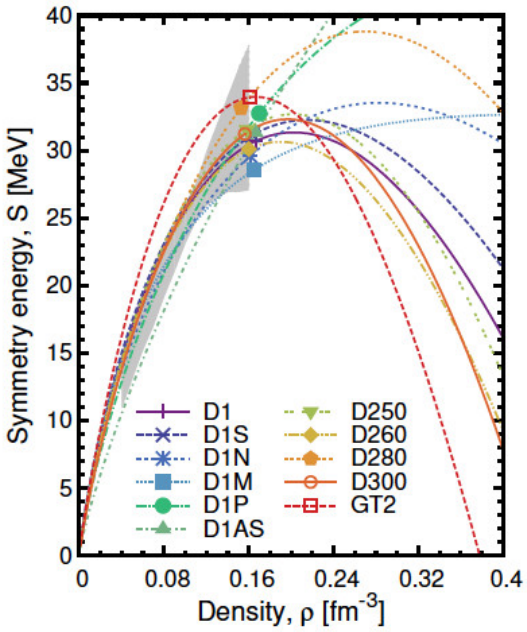

Figure 4.9: Symmetry energy as a function of density for all Gogny interactions. Taken from Ref. [12]

Exercise 12

Calculate the HF energy per particle using the following interaction in a spin and isospin saturated system (Symmetric Nuclear Matter). No Coulomb interaction.

$$V = \sum_{i=1}^{2} [W_i + B_i P_\sigma - H_i P_\tau - M_i P_\sigma P_\tau] \, e^{-(r/\mu_i^C)^2} + t^{(DD)}(1 + x^{(DD)} P_\sigma)\rho^\alpha(\mathbf{R})\delta(\mathbf{r})$$

Note you do not need to use explicit values for $W_i, B_i, \ldots...$

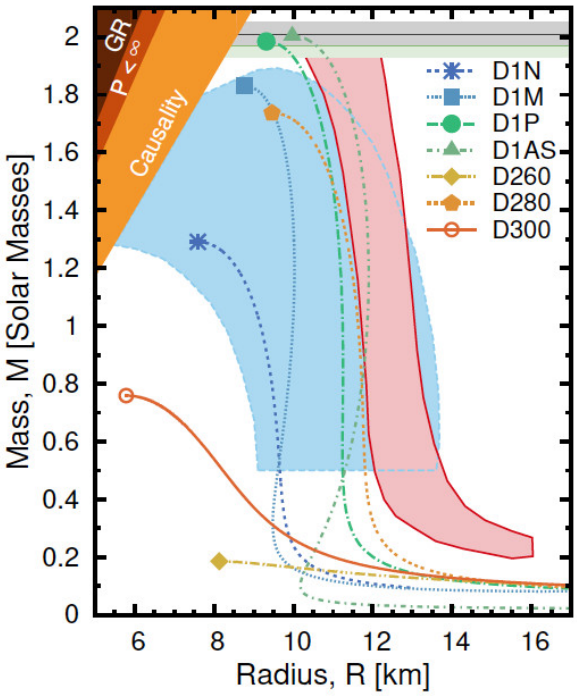

Figure 4.10: Mass-radius relation for neutron stars obtained with 11 Gogny interaction. The shaded region enclosed by a full line is obtained from quiescent low-mass X ray binary mass and radius observations using atmosphere models that include both hydrogen and helium. The upper limit on NS mass is indicated by a grey line.Taken from Ref. [12]

Lecture 5

Spontaneous symmetry breaking [Week 1, day 5]

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5.1 Spontaneous breaking of parity symmetry in ammonia molecule

The Lennard-Jones potential, which describes the atom-atom interaction in a diatomic molecule, has the form:

$$V(r) = \epsilon \left[\left(\frac{r_m}{r} \right)^{12} - 2 \left(\frac{r_m}{r} \right)^{6} \right], \tag{5.1}$$

where r_m is the distance between atoms.

The binding energy of the molecule with bond lengths NH and HH $r_{\rm NH}$ and $r_{\rm HH}$ respectively is equal to:

$$\begin{aligned} E_{\rm NH_3}(r_{\rm NH}, r_{\rm HH}) &= 3\epsilon_{\rm NH} \left[\left(\frac{d_{\rm NH}}{r_{\rm NH}} \right)^{12} - 2 \left(\frac{d_{\rm NH}}{r_{\rm NH}} \right)^{6} \right] \\ &\quad + 3\epsilon_{\rm HH} \left[\left(\frac{d_{\rm HH}}{r_{\rm HH}} \right)^{12} - 2 \left(\frac{d_{\rm HH}}{r_{\rm HH}} \right)^{6} \right], \end{aligned} \tag{5.2}$$

where $d_{\rm NH}$ and $d_{\rm HH}$ are the bond lengths in equilibrium.

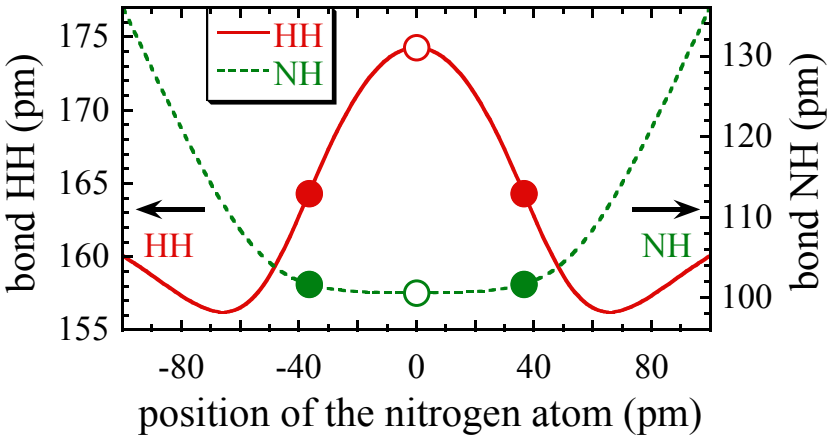


Figure 5.1: HH bond length (solid line, left axis) and NH bond length (dotted line, right axis) obtained from the energy minimization (5.2) at a predetermined position of the nitrogen atom d. Filled circles indicate the bond lengths in the actual molecule of ammonia and the empty circles correspond to a hypothetical flat molecule.

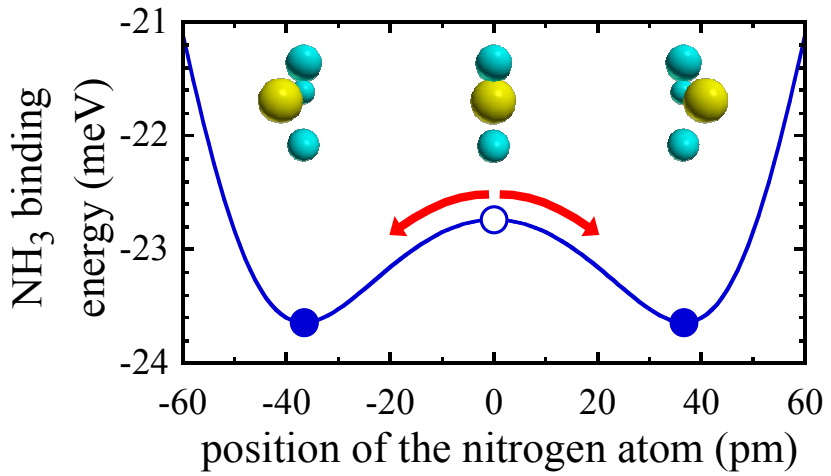


Figure 5.2: The binding energy of the molecule of ammonia as a function of the position of the nitrogen atom d. Filled circles represent the energies of bonds in the actual molecule of ammonia, and the empty circle corresponds to a hypothetical flat molecule.

Let us denote overlaps and Hamiltonian matrix elements in the two-dimensional Hilbert space

by

$$\begin{aligned} 1 &= \langle L|L\rangle = \langle R|R\rangle, && (5.3a)\\ \epsilon &= \langle L|R\rangle = \langle R|L\rangle, && (5.3b)\\ E_0 &= \langle L|\hat{H}|L\rangle = \langle R|\hat{H}|R\rangle, && (5.3c)\\ \Delta &= \langle L|\hat{H}|R\rangle = \langle R|\hat{H}|L\rangle. && (5.3d) \end{aligned}$$

In the non-orthogonal basis of states $|L\rangle$ and $|R\rangle$, the Hamiltonian H and overlap N matrices read,

$$H = \begin{pmatrix} E_0 & \Delta \\ \Delta & E_0 \end{pmatrix}, \qquad N = \begin{pmatrix} 1 & \epsilon \\ \epsilon & 1 \end{pmatrix}, \tag{5.4}$$

and the orthogonal eigenstates can be very easily found:

$$|\pm\rangle = \frac{1}{\sqrt{2 \pm 2\epsilon}} \left(|L\rangle \pm |R\rangle \right), \tag{5.5}$$

with

$$\hat{P}|\pm\rangle = \pm|\pm\rangle, \tag{5.6}$$

and correspond to eigenenergies

$$E_\pm = \langle \pm|\hat{H}|\pm\rangle = \frac{E_0 \pm \Delta}{1 \pm \epsilon}. \tag{5.7}$$

We thus also see that states $|L\rangle$ and $|R\rangle$ are not eigenstates, but linear combinations thereof, that is, wave packets:

$$\begin{aligned} |L\rangle &= \frac{1}{2}\left(\sqrt{2+2\epsilon}|+\rangle + \sqrt{2-2\epsilon}|-\rangle \right), && (5.8a)\\ |R\rangle &= \frac{1}{2}\left(\sqrt{2+2\epsilon}|+\rangle - \sqrt{2-2\epsilon}|-\rangle \right). && (5.8b) \end{aligned}$$

It is very useful to understand states $|\pm\rangle$ as projected or symmetry-restored states. Indeed, we can define projection operators on both parities as

$$\Pi_\pm = \tfrac{1}{2}(1 \pm \hat{P}), \qquad \Pi_\pm^2 = \Pi_\pm, \tag{5.9}$$

in terms of which,

$$|\pm\rangle = N_\pm \Pi_\pm |L\rangle = \pm N_\pm \Pi_\pm |R\rangle, \tag{5.10}$$

where $N_\pm$ are normalization constants.

As a next step, we will carry out a diagonalization of Hamiltonian (5.4) for all values of the parameter d, assuming that

$$\begin{aligned} E_0(d) &= E_{\mathrm{NH_3}}(d), && (5.11a)\\ \epsilon(d) &= \exp\left(-\tfrac{1}{2}a^2(2d)^2\right), && (5.11b)\\ \Delta(d) &= \left(h_0 - \tfrac{1}{2}h_2 a^2 (2d)^2\right)\epsilon(d). && (5.11c) \end{aligned}$$

Now, let's consider a T-even observable $\hat{D}$ of negative spatial parity,

$$\hat{D}^+ = \hat{D}, \qquad \hat{T}\hat{D}\hat{T}^+ = \hat{D}, \qquad \hat{P}\hat{D}\hat{P}^+ = -\hat{D}, \tag{5.12}$$

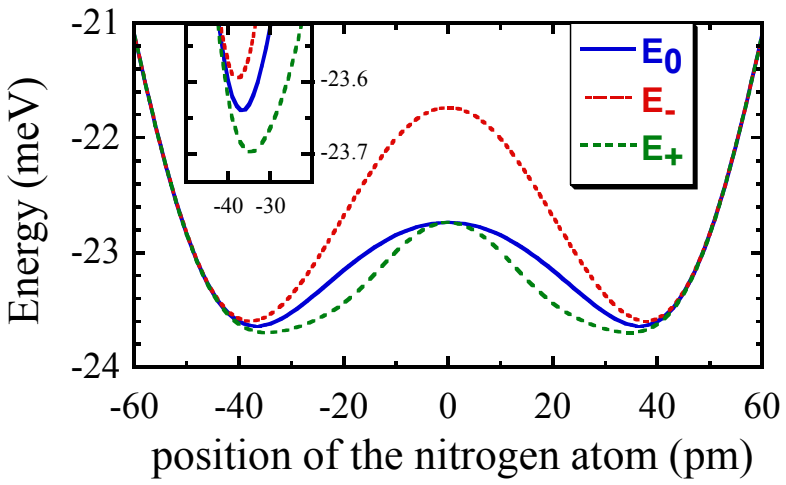


Figure 5.3: Ammonia molecule binding energies as functions of the position of the nitrogen atom d. The solid line represents the binding energy in states, $|L\rangle$ and $|R\rangle$, that break the symmetry (as in Fig. 5.2), and the long-dashed and short-dashed lines correspond to the binding energies E_+ and E_- in the states of the restored symmetry, $|+\rangle$ and $|-\rangle$, respectively. The inset shows the same curves around the minimum in a larger scale.

and assume that we may calculate its matrix elements for states $|L\rangle$ and $|R\rangle$, and therefore also for $|\pm\rangle$ states. An example of such an observable could be the dipole moment of the ammonia molecule, that is, a vector connecting the center of mass of the molecule with the center of its charge. In this case, it only has a non-zero z component, and illustrates the position of the nitrogen atom in relation to the H_3 plane. The matrix of its matrix elements in a non-orthogonal basis of states $|L\rangle$ and $|R\rangle$ has the form of:

$$D = \begin{pmatrix} D_0 & 0 \\ 0 & -D_0 \end{pmatrix}, \tag{5.13}$$

and in an orthogonal basis of states $|\pm\rangle$ it has the form of:

$$D' = \frac{1}{\sqrt{1-\epsilon^2}} \begin{pmatrix} 0 & D_0 \\ D_0 & 0 \end{pmatrix}, \tag{5.14}$$

where $D_0 \equiv \langle L|\hat{D}|L\rangle$, see problem 12.

The squared module of the matrix element $\langle -|\hat{D}|+\rangle$ defines the probability of an E1 transition between the excited negative-parity state $|-\rangle$ and the ground state $|+\rangle$, and so we know its experimental value:

$$\mathrm{B\,(E1;}|-\rangle \to |+\rangle) \sim |\langle -|\hat{D}|+\rangle|^2 = \frac{D_0^2}{1-\epsilon^2} = (30.6)^2\,\mathrm{e}^2\,\mathrm{pm}^2. \tag{5.15}$$

$$|\langle -|\hat{D}|+\rangle|^2 = \frac{(0.836\,\mathrm{e})^2 d^2}{1-\exp\left(-a^2(2d)^2\right)} \xrightarrow[d\,\to\,0]{} \frac{(0.836\,\mathrm{e})^2}{4a^2} = (10.0)^2\,\mathrm{e}^2\,\mathrm{pm}^2. \tag{5.16}$$

So, had the ammonia molecule been flat (d=0), the probability of the E1 transition $|-\rangle \to |+\rangle$ would have been ten times smaller than experimentally observed.

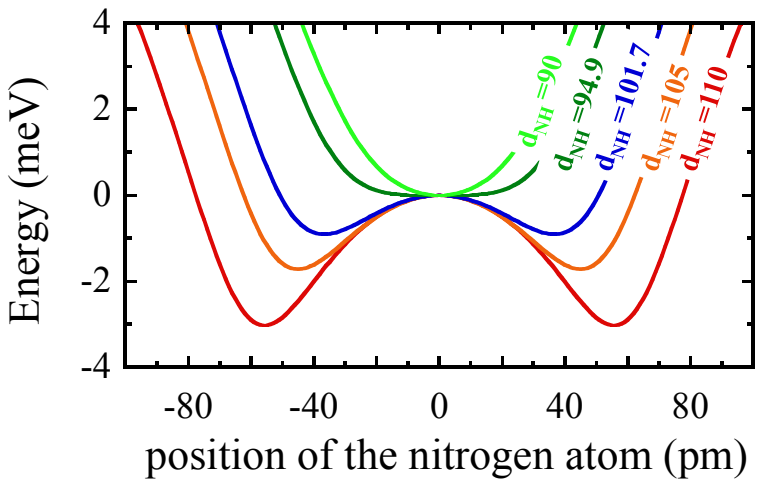


Figure 5.4: The binding energies in the ammonia molecule in the symmetry breaking states $|L\rangle$ and $|R\rangle$ plotted as a function of the position of the nitrogen atom d. The following curves represent the solutions for different lengths of d_{NH} bonds.

5.2 Self-consistent symmetries

According to the nature of nuclear interactions, the nuclear Hamiltonian has six basic symmetries:

1° translational symmetry,

2° rotational symmetry,

3° isospin symmetry,

4° particle-number symmetry,

5° space-parity symmetry,

6° time-reversal symmetry.

Discrete symmetries, Signature:

$$\hat{R}_k := e^{-i\pi \hat{I}_k}, \quad \hat{R}_k^2 = (-1)^A, \tag{5.17}$$

where $\hat{I}_k$ is the operator of the projection of the total angular momentum on the kth axis.

Simplex:

$$\hat{S}_k := \hat{P}\hat{R}_k, \quad \hat{S}_k^2 = (-1)^A. \tag{5.18}$$

The simplexes are nothing but mirror reflections with respect to planes y-z, z-x, and x-y, for $k = x, y, z$, respectively.

Continuous symmetries:

$$\hat{U} = \exp\left(i\alpha\hat{S}\right) \quad \text{or} \quad \hat{U} = \exp\left(i\boldsymbol{\alpha}\cdot\hat{\boldsymbol{S}}\right). \tag{5.19}$$

Hermitian operators $\hat{S}$ (or $\hat{\boldsymbol{S}}$) are called generators of symmetry operators $\hat{U}$, and, for the above mentioned symmetries, they are:

1° total momentum operator: $\hat{\boldsymbol{P}}=\sum_{i=1}^{A}\boldsymbol{p}_i$,

2° total angular-momentum operator: $\hat{\boldsymbol{I}}=\sum_{i=1}^{A}\boldsymbol{j}_i$,

3° total isospin operator: $\hat{\boldsymbol{T}}=\sum_{i=1}^{A}\boldsymbol{t}_i$,

4° particle number operator $\hat{N}$,

8° total position operator: $\hat{\boldsymbol{R}}=\sum_{i=1}^{A}\boldsymbol{r}_i$,

where $\boldsymbol{p}_i$, $\boldsymbol{j}_i$, $\boldsymbol{t}_i$ and $\boldsymbol{r}_i$ are, respectively, operators of momentum, angular momentum, isospin and coordinates of the i-th particle.

The parameters of the above continuous symmetries are, respectively,

1° $\boldsymbol{\alpha}_r=-\boldsymbol{r}_0/\hbar$, where $\boldsymbol{r}_0$ is the vector of translation,

2° $\boldsymbol{\alpha}_n=-\boldsymbol{n}_0/\hbar$, where $|\boldsymbol{n}_0|$ is the angle of rotation around axis $\boldsymbol{n}_0/|\boldsymbol{n}_0|$,

3° $\boldsymbol{\alpha}_m=-\boldsymbol{m}_0/\hbar$, where $|\boldsymbol{m}_0|$ is the angle of rotation in isospace around axis $\boldsymbol{m}_0/|\boldsymbol{m}_0|$,

4° $\alpha_\phi = -\phi_0/\hbar$, where ϕ_0 is the so-called gauge angle,

8° $\boldsymbol{\alpha}_v=-m\boldsymbol{v}_0/\hbar$, where $\boldsymbol{v}_0$ is the change of the system velocity.

All continuous symmetries discussed here are one-body symmetries, that is, their generators are one-body operators,

$$\hat{S} = \sum_{\mu\nu} S_{\mu\nu} a^+_\mu a_\nu. \tag{5.20}$$

$$\hat{U} a_\mu \hat{U}^+ = \sum_{\nu} U^+_{\mu\nu} a_\nu, \tag{5.21}$$

where matrix U is directly connected with matrix S:

$$U = \exp\left(i\alpha S\right). \tag{5.22}$$

5-1: Theorem about self-consistent symmetries

If operator $\hat{U}$ is a one-body symmetry of Hamiltonian $\hat{H}$, that is,

$$\hat{U}\hat{H}\hat{U}^{+} = \hat{H}, \tag{5.23}$$

then one-body Hamiltonian $h[\rho]$, induced by density matrix ρ, has the property:

$$Uh[\rho]U^{+} = h[U\rho U^{+}]. \tag{5.24}$$

If the density matrix is invariant with respect to the given symmetry, thus $U\rho U^{+}=\rho$, theorem (5.24) says that also the induced Hamiltonian is invariant with respect to this symmetry,

$$U\rho U^{+} = \rho \quad \Longrightarrow \quad UhU^{+} = h. \tag{5.25}$$

This implication, written for the symmetry generator and self-consistent density matrix, has the form:

$$[S, \rho_0] = 0 \quad \Longrightarrow \quad [S, h_0] = 0. \tag{5.26}$$

The theorem about self-consistent symmetries 5-1 does not say if the self-consistent solution is, or is not invariant with respect to the given symmetry. In general, depending on the interaction, we may obtain solutions that do, or do not have symmetries of the many-body Hamiltonian:

5-2: Broken symmetries

Solutions of the Hartree-Fock equations do not have to have all symmetries of the Hamiltonian of the system. We will call a self-consistent solution that is not invariant with respect to the given symmetry, broken-symmetry solution or symmetry-breaking solution.

5-3: Interpretation of broken symmetries

Symmetry-breaking solutions of the Hartree-Fock equations should be interpreted as approximations of wave packets, and not as approximations of exact eigenstates of the Hamiltonian.

5.3 Spontaneous breaking of other symmetries

In the case of rotational symmetry the order operator is the quadrupole-moment tensor,

$$\hat{Q}_{\mu} = \sum_{i=1}^{A} r_i^2 Y_{2\mu}(\theta_i, \phi_i), \tag{5.27}$$

where r_i, θ_i, ϕ_i are the coordinates of the ith nucleon in a spherical coordinate system and $Y_{2\mu}$ are standard spherical harmonics (spherical functions) [13, 14]. This operator defines the probabilities of electromagnetic quadrupole transitions E2 and is the order operator for the rotational-symmetry breaking.

Particle-number-symmetry breaking aims at describing the deviations of the exact density matrix from a projective density matrix without going outside the class of product states. For this symmetry breaking, the order operator could be the operator of the collective-pair transfer.

$$\hat{P} = \sum_{\nu} s_\nu u_\nu v_\nu \bar{a}^+_{\tilde{\nu}} \bar{a}^+_\nu, \tag{5.28}$$

but an equally good one could be the operator of the dispersion of the particle number squared,

$$\hat{\sigma}^2_N = \hat{N}^2 - \langle \Phi | \hat{N} | \Phi \rangle^2 \tag{5.29}$$

.

In nuclei having a particular shell structure [15], with large orbitals of opposite parity on two sides of the Fermi energy, the symmetry of spatial parity will be spontaneously broken. For such a symmetry breaking, a proper order operator is the isovector-dipole-moment operator,

$$\hat{Q}^{\mathrm{IV}}_{1\mu} = \sum_{i=1}^{A} \hat{\tau}^z_i r_i Y_{1\mu}(\theta_i, \phi_i), \tag{5.30}$$

cf. Eq. (5.27), where $\hat{\tau}^z$ is a doubled third component of the isospin (equals $+1$ for neutrons and -1 for protons). An equally good order operator is also the isoscalar octupole moment operator

$$\hat{Q}^{\mathrm{IS}}_{3\mu} = \sum_{i=1}^{A} r^3_i Y_{3\mu}(\theta_i, \phi_i), \tag{5.31}$$

which measures the "pear-shape" of the nucleus.

5.4 The Goldstone theorem

Each self-consistent solution that breaks a given symmetry allows us to give a whole class of self-consistent solutions. For if

$$\rho_0 \neq \rho'_0 = U \rho_0 U^+, \tag{5.32}$$

then for $h'_0 = h[\rho'_0]$, from the theorem about self-consistent symmetries, we have

$$[h'_0, \rho'_0] = [U h_0 U^+, U \rho_0 U^+] = U[h_0, \rho_0] U^+ = 0. \tag{5.33}$$

5-4: The Goldstone Theorem

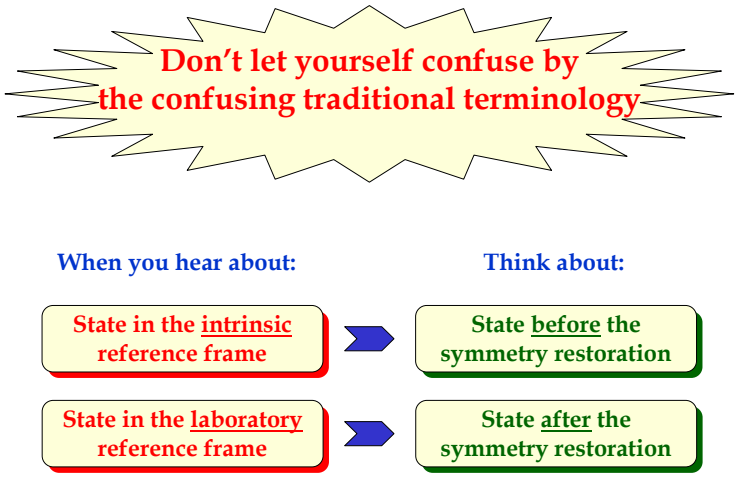
If the self-consistent solution ρ_0 breaks a continuous one-body symmetry with the generator given by matrix S, formula (5.20), then matrix

$$\rho_1^S := i[S, \rho_0] \tag{5.34}$$

is the eigenvector of stability operator $\mathtt{M}_0$ of this self-consistent solution with an eigenvalue of zero, thus

$$\mathtt{M}_0 \rho_1^S = 0. \tag{5.35}$$

5.5 Take-away messages



5.6 Exercises

Exercise 12.

Prove that the matrix elements D of the order operator $\hat{D}$ (5.12) in the symmetry-breaking states $|L\rangle$ and $|R\rangle$ have the form (5.13), and those D' in the symmetry-restored states $|\pm\rangle$ have the form (5.14).

Exercise 13.

Consider two exact eigenstates of the Hamiltonian, $|+\rangle_{\rm exact}$ and $|-\rangle_{\rm exact}$, which have opposite parities, small excitation energy, $\Delta E^{\rm exact} = E_-^{\rm exact} - E_+^{\rm exact}$, and large E1 transition matrix element, $D_0^{\rm exact} = {}_{\rm exact}\langle -|\hat{D}|+\rangle_{\rm exact}$. Use them to construct two exact wave packets,

$$\begin{aligned} |L\rangle_{\rm exact} &= \cos(\alpha)|+\rangle_{\rm exact} \\ &+ \sin(\alpha)|-\rangle_{\rm exact}, \end{aligned} \tag{5.36a}$$

$$\begin{aligned} |R\rangle_{\rm exact} &= \cos(\alpha)|+\rangle_{\rm exact} \\ &- \sin(\alpha)|-\rangle_{\rm exact}. \end{aligned} \tag{5.36b}$$

In function of the mixing angle α determine the exact matrix elements defined in Eqs. (5.3) and show for which mixing angles: 1° average energies of these two wave packets are equal. 2° average dipole moments of these two wave packets have opposite signs. 3° overlaps between these two wave packets are small. 4° Hamiltonian matrix elements between these two wave packets are small. Also determine the Hamiltonian kernel, $\Delta(\alpha)/\epsilon(\alpha)$, and discuss the question of how one can reconcile this result with the Gaussian overlap approximation (5.11c).

Exercise 14.

Prove that average energies of all symmetry-breaking Hartree-Fock states that are transformed by the symmetry operator are all equal.

Exercise 15.

Prove the Goldstone theorem 5-4, see Ref. [16].

Lecture 6

Spontaneous Symmetry Breaking II: Pairing Correlations [Week 2 day 1]

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6.1 Wick theorem for General Product States

Assume generic fermionic operators $\{\beta, \beta^\dagger\}$. Usual anticommutation relations are

$$\{\beta_\mu^\dagger, \beta_\nu^\dagger\} = 0, \quad \{\beta_\mu, \beta_\nu\} = 0, \quad \{\beta_\mu, \beta_\nu^\dagger\} = \delta_{\mu\nu} \tag{6.1}$$

Define product state from said operators as

$$|\Phi\rangle = \prod_\mu \beta_\mu |0\rangle \tag{6.2}$$

where $|0\rangle$ is the particle vacuum (here we do not have $\beta_\mu|0\rangle = 0$)

To use Wick theorem for $\langle\Phi|\hat{A}\hat{B}|\Phi\rangle/\langle\Phi|\Phi\rangle$ with $\hat{A}$, $\hat{B}$ expressed in terms of the fermionic operator a_k, we need

$$a_k = a_{k0} + a_{k+} + a_{k-} \tag{6.3}$$

How can we express operators a_{k0}, a_{k+} and a_{k-} in terms of the $\{a, a^\dagger\}$?

Generic form for the annihilation operator

$$a_{k-} = \sum_{mn} \hat{T}(m,n) \tag{6.4}$$

where

$$\hat{T}(m,n) = \sum_\alpha C_\alpha a_1^\dagger \cdots a_m^\dagger a_1 \cdots a_n \tag{6.5}$$

6-1: Wick Theorem for Product States

The contractions $\overbrace{a_k a_l^\dagger}$ and $\overbrace{a_k a_l}$ (and $\overbrace{a_k^\dagger a_l^\dagger}$ and $\overbrace{a_k^\dagger a_l}$) are numbers if and only if a_{k-} and a_{k+} (and $a_{k-}^\dagger$ and $a_{k+}^\dagger$) are linear combinations of creation and annihilation operators. For a_{k-},

$$\begin{aligned} a_{k-} &= \sum_l X_{kl} a_l + \sum_l Y_{kl} a_l^\dagger \\ a_{k-}^\dagger &= \sum_l X'_{kl} a_l + \sum_l Y'_{kl} a_l^\dagger \end{aligned} \tag{6.6}$$

By convention (and to anticipate future results), choose the following notations

$$\begin{aligned} X_{kl} &= (1-\rho)_{kl}, & Y_{kl} &= -\kappa_{kl} \\ X'_{kl} &= \kappa'^*_{kl}, & Y'_{kl} &= \rho'^T_{kl} \end{aligned} \tag{6.7}$$

Use $a_k = a_{k0} + a_{k+} + a_{k-}$ and the new notations to obtain

$$\begin{aligned} a_{k-} &= \sum_l (1-\rho)_{kl} a_k - \sum_l \kappa_{kl} a_k^\dagger \\ a_{k-}^\dagger &= \sum_l \rho'^T_{kl} a_l^\dagger + \sum_l \kappa'^*_{kl} a_l \end{aligned} \tag{6.8}$$

and

$$\begin{aligned} a_{k+} &= \sum_l \rho_{kl} a_l + \kappa_{kl} a_l^\dagger - x_k \\ a_{k+}^\dagger &= \sum_l (1-\rho'^T)_{kl} a_l^\dagger - \sum_l \kappa'^*_{kl} a_l - y_k^* \end{aligned} \tag{6.9}$$

where $x_k = \overbrace{a_k}$ and $y_k^* = \overbrace{a_k^\dagger}$

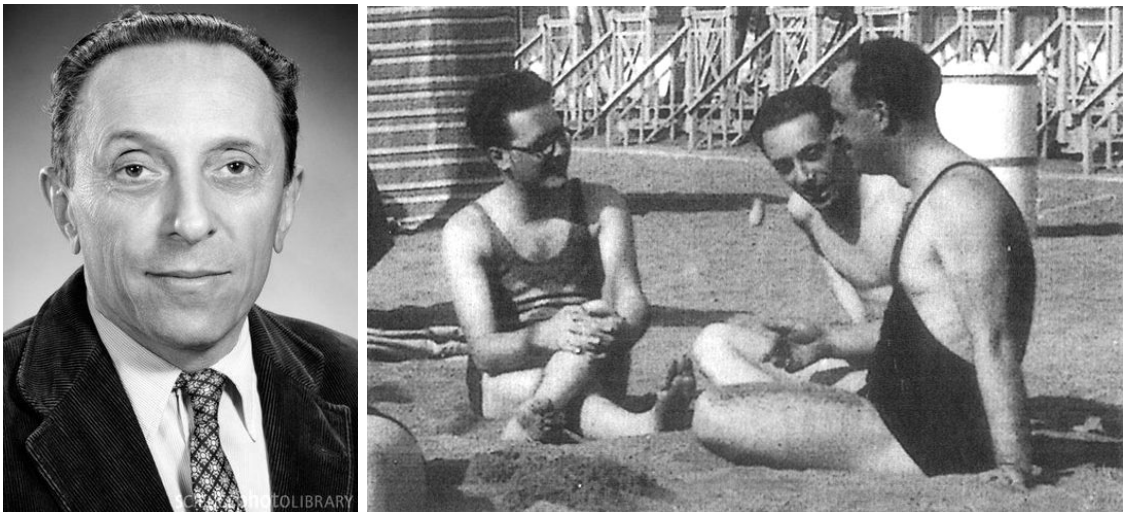

Figure 6.1: **Left: Gian Carlo Wick (1909-1992). Right: Wick and Fermi brainstorming on Ostia beach**

Wick contractions are then defined as

$$\begin{array}{lll} \overbrace{a_k^\dagger a_l} & = \{a_{k-}^\dagger, a_l\} & = \rho_{kl}'^T, \\ \overbrace{a_k a_l} & = \{a_{k-}, a_l\} & = -\kappa_{kl}, \\ \overbrace{a_k a_l^\dagger} & = \{a_{k-}, a_l^\dagger\} & = (1-\rho)_{kl}, \\ \overbrace{a_k^\dagger a_l^\dagger} & = \{a_{k-}^\dagger, a_l^\dagger\} & = \kappa_{kl}'^*. \end{array} \tag{6.10}$$

Anticommutation rules for operators β and $\beta^\dagger$ lead to the relations $x = y = 0$ and

$$\begin{array}{rclcrclcrcl} \rho' & = & +\rho & & \rho^\dagger & = & +\rho & & \rho^2 - \kappa\kappa^* & = & 0 \\ \kappa'^T & = & -\kappa & \text{and} & \kappa^T & = & -\kappa & & \rho\kappa - \kappa\rho & = & 0 \end{array} \tag{6.11}$$

and $x = y = 0$

6.2 The HFB Theory

6.2.1 The Bogoliubov transformation

Bogoliubov transformation

$$\begin{pmatrix} \beta \\ \beta^\dagger \end{pmatrix} = \begin{pmatrix} U^\dagger & V^\dagger \\ V^T & U^T \end{pmatrix} \begin{pmatrix} a \\ a^\dagger \end{pmatrix}, \quad \mathcal{W} = \begin{pmatrix} U & V^* \\ V & U^* \end{pmatrix} \tag{6.12}$$

Unitarity of the Bogoliubov transformation

$$\mathcal{W}\mathcal{W}^\dagger = \mathcal{W}^\dagger\mathcal{W} = 1. \tag{6.13}$$

Figure 6.2: **Left: Nikolay Bogolyubov (1909-1992). Right: Pierre-Gilles de Gennes (1932-2007)**

From particles to quasiparticles (and back)

$$\begin{aligned} \mathcal{W} &: \{\beta, \beta^\dagger\} \to \{a, a^\dagger\} \equiv \langle a|\beta\rangle, \\ \mathcal{W}^\dagger &: \{a, a^\dagger\} \to \{\beta, \beta^\dagger\} \equiv \langle \beta|a\rangle. \end{aligned} \tag{6.14}$$

Quasiparticle (Bogoliubov, HFB) vacuum

$$|\Phi\rangle = \prod_{\mu=1}^{N_p} \beta_\mu |0\rangle, \qquad \forall \mu,\ \beta_\mu|\Phi\rangle = 0 \tag{6.15}$$

with $N_p \leq M$

Quasiparticles represent excitations of the system: the vacuum is the state with no excitation (ground-state). Contrary to HF, HFB gives a recipe for both the g.s. and the excited states.

Quasiparticle operators $\{\beta, \beta^\dagger\}$ are fermionic operators and the HFB vacuum is a product state: general conditions for the Wick theorem apply.

6.2.2 Densities

Given an arbitrary reference state $|\Phi\rangle$, the one-body density matrix is given by

$$\rho_{kl} = \frac{\langle\Phi|a_l^\dagger a_k|\Phi\rangle}{\langle\Phi|\Phi\rangle} = \overbrace{a_l^\dagger a_k}. \tag{6.16}$$

The last equality is only true if $|\Phi\rangle$ is a product state

Similarly, the pairing tensor (abnormal density) is defined as

$$\kappa_{kl} = \frac{\langle\Phi|a_l a_k|\Phi\rangle}{\langle\Phi|\Phi\rangle} = \overbrace{a_l a_k} \tag{6.17}$$

6-2: Densities associated with the HFB vacuum

If the reference state $|\Phi\rangle$ is a HFB vacuum (product state of quasiparticle operators), then

$$\rho = V^* V^T, \quad \kappa = V^* U^T. \tag{6.18}$$

Therefore, there is a one-to-one mapping between the set of densities, the reference state and the matrices of the Bogoliubov transformation

$$|\Phi\rangle \Leftrightarrow (U, V) \Leftrightarrow (\rho, \kappa) \tag{6.19}$$

6-3: Degrees of freedom in the HFB theory

In the HFB theory, the one-body density matrix ρ and the pairing tensor κ encapsulate all the physics degrees of freedom. Since ρ and κ have specific symmetry properties, the actual degrees of freedom are ρ_{kl}, ρ^*_{kl}, κ_{kl}, and κ^*_{kl} for $k \geq l$.

Densities in terms of Wick contractions

$$\begin{aligned} \rho_{kl} &= \overbrace{a_l^\dagger a_k}, \qquad \kappa_{kl} &= \overbrace{a_l a_k}, \\ (1-\rho)^*_{kl} &= \overbrace{a_l a_k^\dagger}, \qquad \kappa^*_{kl} &= \overbrace{a_k^\dagger a_l^\dagger}. \end{aligned} \tag{6.20}$$

Generalized density

$$\mathcal{R} = \begin{pmatrix} \rho & \kappa \\ -\kappa^* & 1-\rho^* \end{pmatrix}, \quad \mathcal{R}^2 = \mathcal{R}, \quad \mathcal{R}^\dagger = \mathcal{R} \tag{6.21}$$

Alternative forms

$$\mathcal{R} = \langle\Phi| \begin{pmatrix} a_l^\dagger a_k & a_l a_k \\ a_l^\dagger a_k^\dagger & a_l a_k^\dagger \end{pmatrix} |\Phi\rangle. \tag{6.22}$$

and

$$\mathcal{R} = \langle\Phi|1 - \mathcal{W} \begin{pmatrix} \beta_\mu \\ \beta_\mu^\dagger \end{pmatrix} (\beta_\nu^\dagger \ \beta_\nu) \mathcal{W}^\dagger |\Phi\rangle = \mathcal{W}\langle\Phi|1 - \begin{pmatrix} \beta_\mu \\ \beta_\mu^\dagger \end{pmatrix} (\beta_\nu^\dagger \ \beta_\nu) |\Phi\rangle \mathcal{W}^\dagger. \tag{6.23}$$

6.2.3 Energies and fields

Hamiltonian version - Traditional mean-field approach based on choosing a (possibly effective) Hamiltonian $\hat{H}$, an ansatz for the reference state $|\phi\rangle$ and computing the energy as

$\langle\Phi|\hat{H}|\Phi\rangle/\langle\Phi|\Phi\rangle$. For the HFB ansatz and a two-body Hamiltonian,

$$E = \sum_{ij} t_{ij}\rho_{ji} + \frac{1}{2}\sum_{ijkl}\bar{v}_{ijkl}\rho_{lj}\rho_{ki} + \frac{1}{4}\sum_{ijkl}\bar{v}_{ijkl}\kappa^*_{ij}\kappa_{kl}. \tag{6.24}$$

Energy density functional version - Simply assume that the energy is now some functional $E[\rho,\rho^*,\kappa,\kappa^*] = E[\mathcal{R}]$ with no necessary connection to a Hamiltonian.

Variational principle for E as a functional of $\mathcal{R}$ (or equivalently of ρ, ρ^*, κ, κ^*) is expressed as

$$\delta E = 0 \Rightarrow \sum_{kl}\frac{\partial E}{\partial\mathcal{R}_{kl}}\delta\mathcal{R}_{kl} = 0 \tag{6.25}$$

Notations

$$\frac{\partial E}{\partial\rho_{kl}} = \frac{1}{2}h_{lk}, \quad \text{and} \quad \frac{\partial E}{\partial\rho^*_{kl}} = \frac{1}{2}h^*_{lk}. \tag{6.26}$$

and

$$\frac{\partial E}{\partial\kappa_{kl}} = \frac{1}{2}\Delta^*_{kl}, \quad \text{and} \quad \frac{\partial E}{\partial\kappa^*_{kl}} = \frac{1}{2}\Delta_{kl}. \tag{6.27}$$

HFB matrix

$$\mathcal{H} = \begin{pmatrix} h & \Delta \\ -\Delta^* & -h^* \end{pmatrix}, \tag{6.28}$$

where the HFB matrix

- is defined by $\frac{1}{2}\mathcal{H}_{kl} = \partial E/\partial\mathcal{R}_{kl}$
- obeys the HFB equation $[\mathcal{H},\mathcal{R}] = 0$
- is such that $\delta E = \frac{1}{2}\mathrm{Tr}(\mathcal{H}\delta\mathcal{R})$

Energy as a functional of $\mathcal{R}$

$$E = \frac{1}{4}\mathrm{tr}\left[(\mathcal{H}+\mathcal{T})\,\mathcal{S}\right], \tag{6.29}$$

with

$$\mathcal{T} = \begin{pmatrix} t & 0 \\ 0 & -t^* \end{pmatrix}, \qquad \mathcal{S} = \begin{pmatrix} \rho & \kappa \\ -\kappa^* & -\rho^* \end{pmatrix} = \mathcal{R} - \begin{pmatrix} 0 & 0 \\ 0 & I_N \end{pmatrix}. \tag{6.30}$$

Generalized eigenvalue problem (non-linear): build the generalized density from the eigenvectors of $\mathcal{H}$ ensures that the commutator equals 0.

Solving the HFB equations determine the generalized density $\mathcal{R}$, hence ρ and κ and *any observable by virtue of the Wick theorem.*

6-4: Quasiparticle basis

The basis that diagonalizes $\mathcal{R}$ (hence $\mathcal{H}$) determines the Bogoliubov transformation matrix $\mathcal{W}$. Alternatively, the vectors

$$\begin{pmatrix} U \\ V \end{pmatrix} \quad \text{and} \quad \begin{pmatrix} V^* \\ U^* \end{pmatrix}, \tag{6.31}$$

are the eigenvectors of both $\mathcal{R}$ and $\mathcal{H}$.

In the case of some two-body potential, the mean field (or Hartree-Fock field) reads

$$h_{kl} = t_{kl} + \Gamma_{kl}, \tag{6.32}$$

with the Hartree-Fock potential (role of a one-body potential)

$$\Gamma_{kl} = \sum_{mn} \bar{v}_{kmln}\rho_{nm} = \sum_{mn} \bar{v}_{mknl}\rho_{nm}. \tag{6.33}$$

and the pairing field

$$\Delta_{kl} = \frac{1}{2}\sum_{mn} \bar{v}_{klmn}\kappa_{mn}, \tag{6.34}$$

6-5: Thouless Theorem Revisited

For a quasiparticle vacuum $|\Phi_0\rangle$ associated with quasiparticles β, $\beta^\dagger$, any other product wave function $|\Phi_1\rangle$ not orthogonal to $|\Phi_0\rangle$ can be written

$$\begin{aligned} &1.\ |\Phi_1\rangle = e^{i\hat{T}}|\Phi_0\rangle, \\ &2.\ \hat{T} = \sum_{\mu<\nu} T_{\mu\nu}\beta^\dagger_\mu\beta^\dagger_\nu + \sum_{\mu<\nu} T^\dagger_{\mu\nu}\beta_\mu\beta_\nu. \end{aligned} \tag{6.35}$$

In other words, the matrix of the transformation $\hat{T}$ in the q.p. basis associated with the state $|\Phi_0\rangle$ takes the generic form

$$\tilde{T} = \begin{pmatrix} 0 & T^\dagger \\ T & 0 \end{pmatrix}. \tag{6.36}$$

Application: Collective momentum. Suppose $|\Phi_0\rangle \equiv |\Phi(\mathbf{a})\rangle$ and $|\Phi_1\rangle \equiv |\Phi(\mathbf{a}+\delta\mathbf{a})\rangle$. Since we must have $\lim_{\delta\mathbf{a}\to 0}|\Phi_1\rangle = |\Phi_0\rangle$, choose the transformation $\hat{T}$ in the form $\hat{T} = \delta\mathbf{a}\cdot\hat{\mathbf{P}}_\mathbf{a}/\hbar$. We have

$$\lim_{\delta\mathbf{a}\to 0}\left(\frac{|\Phi(\mathbf{a}+\delta\mathbf{a})\rangle - |\Phi(\mathbf{a})\rangle}{\delta\mathbf{a}}\right) \equiv \frac{\partial}{\partial\mathbf{a}}|\Phi(\mathbf{a})\rangle = \frac{i}{\hbar}\hat{\mathbf{P}}_\mathbf{a}|\Phi(\mathbf{a})\rangle. \tag{6.37}$$

and therefore $\hat{\mathbf{P}}_\mathbf{a} = -i\hbar\frac{\partial}{\partial\mathbf{a}}$

Application: Multi-reference EDF and symmetry restoration.

$$\rho_{ij}^{01} = \frac{\langle \Phi_1 | c_j^\dagger c_i | \Phi_0 \rangle}{\langle \Phi_1 | \Phi_0 \rangle} \tag{6.38}$$

where $|\Phi_0\rangle$ correspond to a HFB vacuum for some collective variable $\boldsymbol{q}$ or gauge angle $\boldsymbol{\alpha}$ and $|\Phi_1\rangle$ correspond to a different HFB vacuum with $\boldsymbol{q}'$ or $\boldsymbol{\alpha}'$.

6.3 The BCS Approximation

Figure 6.3: **Left to right: John Bardeen (1908-1991), Leon Cooper (1930-), Robert Schrieffer (1931-).**

6.3.1 General Case

6-6: Bloch-Messiah Theorem

A unitary matrix $\mathcal{W}$ of the form (6.12) can always be decomposed as follows

$$\mathcal{W} = \begin{pmatrix} D & 0 \\ 0 & D^* \end{pmatrix} \begin{pmatrix} \bar{U} & \bar{V} \\ \bar{V} & \bar{U} \end{pmatrix} \begin{pmatrix} C & 0 \\ 0 & C^* \end{pmatrix} \tag{6.39}$$

where $\bar{U}$ and $\bar{V}$ are in the canonical form

$$\bar{U} = \begin{pmatrix} 0 & & & & & 0 \\ & \ddots & & & & \\ & & u_k & 0 & & \\ & & 0 & u_{\bar{k}} & & \\ & & & & \ddots & \\ 0 & & & & & 1 \end{pmatrix}, \quad \bar{V} = \begin{pmatrix} 1 & & & & & 0 \\ & \ddots & & & & \\ & & 0 & v_k & & \\ & & v_{\bar{k}} & 0 & & \\ & & & & \ddots & \\ 0 & & & & & 0 \end{pmatrix},$$

Interpretation of the Bloch-Messiah theorem

$$\mathcal{W} : \{\beta\} \to \{a\} = \{\beta\} \overset{C}{\to} \{\alpha\} \overset{\bar{U},\bar{V}}{\to} \{c\} \overset{D}{\to} \{a\}. \tag{6.40}$$

- Transforms quasi-particle operators into themselves: transformation C;
- Goes from the quasi-particle basis to a particle-basis: transformation $(\bar{U}, \bar{V})$;
- Transforms the particle operators into themselves: transformation D.

6-7: Canonical Basis

The transformation D diagonalizes the density matrix ρ and puts the pairing tensor κ into the canonical form analogous of $\bar{V}$. This transformation defines the *canonical* basis.

In the canonical basis, the HFB vacuum reads

$$|\Phi\rangle = \prod_k \alpha_k |0\rangle = \prod_{k>0} \alpha_k \alpha_{\bar{k}} |0\rangle \tag{6.41}$$

Special Bogoliubov transformation $(\bar{U}, \bar{V})$

$$\begin{aligned} \alpha_k^\dagger &= u_k c_k^\dagger + v_{\bar{k}} c_{\bar{k}}, & \alpha_k &= u_k^* c_k + v_{\bar{k}}^* c_{\bar{k}}^\dagger, \\ \alpha_{\bar{k}}^\dagger &= u_{\bar{k}} c_{\bar{k}}^\dagger + v_k c_k, & \alpha_{\bar{k}} &= u_{\bar{k}}^* c_{\bar{k}} + v_k^* c_k^\dagger. \end{aligned} \tag{6.42}$$

Additionally:

$$(u_k, v_k) \in \mathbb{R}^2, \quad u_{\bar{k}} = u_k, \quad v_{\bar{k}} = -v_k \tag{6.43}$$

6-8: BCS wave function

Given an arbitrary single-particle basis characterized by operators c_k, the ansatz for the many-body wave function for an even-even system is

$$|\phi\rangle = \prod_{k>0} \left(u_k + v_k c_k^\dagger c_{\bar{k}}^\dagger\right)|0\rangle \tag{6.44}$$

with

- $|0\rangle$ is the particle-vacuum, $c_k|0\rangle = 0, \forall k$
- $|\bar{k}\rangle = \hat{T}|k\rangle$ time-reversed partner of state $|k\rangle$ and the product runs only over states k
- $|u_k|^2 + |v_k|^2 = 1$

Energy (with constraint on particle number) assuming ansatz (6.44),

$$E[\rho, \kappa, \kappa^*] = \frac{1}{2}\sum_k v_k^2(h_{kk} + t_{kk} - \lambda) + \frac{1}{2}\sum_{k>0} \Delta_{k\bar{k}} u_k v_k \tag{6.45}$$

Variational principle implemented using derivatives with respect to u_k and v_k keeping in mind that $u_k^2 + v_k^2 = 1$, hence $du_k/dv_k = -v_k/u_k$ yields

$$\begin{aligned} 2(h_{kk} + t_{kk} - \lambda)u_k v_k + \frac{1}{2}\Big[&\Delta_{k\bar{k}} + \Delta^*_{k\bar{k}} \\ &+4\sum_{m>0} \frac{\partial^2 E}{\partial \kappa^*_{m\bar{m}} \partial \kappa_{k\bar{k}}} u_m v_m + 4\sum_{m>0} \frac{\partial^2 E}{\partial \kappa_{m\bar{m}} \partial \kappa^*_{k\bar{k}}} u_m v_m\Big](u_k^2 - v_k^2) = 0 \end{aligned} \tag{6.46}$$

Special case: pairing force such that

$$4\frac{\partial^2 E}{\partial \kappa^*_{m\bar{m}} \partial \kappa_{k\bar{k}}} = \bar{v}_{k\bar{k}m\bar{m}} \tag{6.47}$$

yields the gap equation

$$\Delta_{k\bar{k}} = \sum_{m>0} \bar{v}_{k\bar{k}m\bar{m}} u_m v_m = -\Delta_k \quad (k > 0) \tag{6.48}$$

6.3.2 Seniority pairing: constant pairing strength

Assume a pairing force characterized by

$$v_{\alpha\beta\gamma\delta} = -\frac{1}{4} G \delta_{\alpha\bar{\beta}} \delta_{\gamma\bar{\delta}} \,\mathrm{sign}(\alpha)\mathrm{sign}(\gamma) \tag{6.49}$$

Pairing gap is constant and reads

$$\Delta_{\mu\nu} = -\mathrm{sign}(\mu)\delta_{\mu\nu}\Delta, \qquad \Delta = G\sum_{\mu>0} \kappa_{\mu\bar{\mu}} = G\sum_{\mu>0} u_\mu v_\mu \tag{6.50}$$

Gap equation

$$\Delta = \frac{G}{2}\sum_{\mu>0}\frac{\Delta}{\sqrt{(e_\mu-\lambda)^2+\Delta^2}} \tag{6.51}$$

Pairing energy

$$E_{\text{pair}} = -\frac{\Delta^2}{G} + G\sum_{\mu>0} v_\mu^4 \tag{6.52}$$

Quasiparticle energy

$$E_k = \sqrt{(e_k-\lambda)^2+\Delta^2} \tag{6.53}$$

Occupations

$$u_k^2 = \frac{1}{2}\left(1+\frac{e_k-\lambda}{\Gamma_k}\right); \qquad v_k^2 = \frac{1}{2}\left(1-\frac{e_k-\lambda}{\Gamma_k}\right) \tag{6.54}$$

6.3.3 Odd Nuclei

Suppose one state k is not paired with $\bar{k}$. If $v_k = 1$, then $u_k = 0$, but also $v_{\bar{k}} = 0$ and $u_{\bar{k}} = 1$. Then $\alpha_k\alpha_{\bar{k}} = c_{\bar{k}}^\dagger c_k \Rightarrow \alpha_k\alpha_{\bar{k}}|0\rangle = 0$

HFB theory as presented above always produces fully paired vacua, which involve only superposition of eigenstates of $\hat{N}$ with even particle number

$$|\Phi\rangle = \sum_N c_{2N}|2N\rangle \tag{6.55}$$

Modification: describe odd nucleus as a 1 qp excitation of an even-even (fully-paired) system

$$|\Phi\rangle_{\text{odd}} = \beta_{\mu_0}^\dagger|\Phi\rangle_{\text{eve}}. \tag{6.56}$$

Odd-nucleus HFB vacuum

$$|\Phi\rangle_{\text{odd}} = \prod_\mu \tilde{\beta}_\mu|0\rangle, \quad \{\tilde{\beta}\} = \{\tilde{\beta}_1 = \beta_1, \ldots, \tilde{\beta}_{\mu_0} = \beta_{\mu_0}^\dagger, \ldots \tilde{\beta}_M = \beta_M\}, \tag{6.57}$$

In practice, at each iteration of the HFB equation, substitute

$$\begin{array}{l} U_{i\mu_0} \to V_{i\mu_0}^*, \quad \forall i, \\ V_{i\mu_0} \to U_{i\mu_0}^*, \quad \forall i. \end{array} \tag{6.58}$$

6.4 Projection on Good Particle Number

6.4.1 U(1) Symmetry Breaking

Back to Slater determinant $|\Phi\rangle$, by definition

$$\hat{N}|\Phi\rangle = N|\Phi\rangle \Rightarrow |\Phi'\rangle \equiv e^{-i\phi\hat{N}}|\Phi\rangle = e^{-i\phi N}|\Phi\rangle \tag{6.59}$$

and all densities $\rho_\phi \propto \langle\Phi'|a^\dagger a|\Phi'\rangle$ are identical, hence all energies $E[\rho_\phi]$ are degenerate.

Transformation

$$\mathcal{U}_\phi : |\Phi\rangle \mapsto |\Phi'\rangle \equiv e^{-i\phi\hat{N}}|\Phi\rangle \tag{6.60}$$

is an example of a U(1) symmetry group.

HFB (and BCS) states are not invariant under transformation $\mathcal{U}_\phi$: symmetry is broken

- There is an *order parameter* g that characterizes the degree to which symmetry is broken ($g = 0$ for symmetry-conserved states)
- The order parameter is a complex number of the form $g = |g|e^{i\alpha}$, with $|g|$ measures the "deformation" and α the "orientation".

For particle number symmetry, $|g|$ could be anything related to, e.g., κ, Δ, $\langle\Delta\hat{N}^2\rangle$; ϕ as in (6.59) is a good choice for the phase α as it is the angle that defines a particle-number rotation in Fock space.

6.4.2 Symmetry Restoration

Particle number projection operator

$$\hat{P}^N = \frac{1}{2\pi}\int_0^{2\pi} d\phi e^{i\phi(\hat{N}-N)}, \tag{6.61}$$

Projected density

$$\rho^N_{ji} = \frac{\langle\Phi|c_i^\dagger c_j \hat{P}^N|\Phi\rangle}{\langle\Phi|\hat{P}^N|\Phi\rangle} = \frac{1}{2\pi}\int_0^{2\pi} d\phi\, y(\phi)\frac{\langle\Phi|c_i^\dagger c_j e^{i\phi(\hat{N}-N)}|\Phi\rangle}{\langle\Phi|e^{i\phi(\hat{N}-N)}|\Phi\rangle} = \frac{1}{2\pi}\int_0^{2\pi} d\phi\, y(\phi)\rho_{ji}(\phi) \tag{6.62}$$

with $|\Phi\rangle$ a symmetry-breaking state (Bogoliubov vacuum)

Two alternatives here

- Express the energy functionals $E[\rho^N, \kappa^N]$, calculate the corresponding HFB matrix by taking partial (functional) derivatives with respect to ρ^N and κ^N: Variation After Projection (VAP)
- Solve HFB equations as usual and *at convergence*, calculate $E[\rho^N, \kappa^N]$: Projection After Variation (PAV)

Key is the possibility to compute transition densities $\rho(\phi)$, etc. from only the knowledge of the Bogoliubov transformation. Define the matrices

$$\begin{aligned} N^{11} &= U^\dagger U - V^\dagger V, \\ N^{20} &= U^\dagger V^* - V^\dagger U^*, \\ N^{02} &= V^T U - U^T V. \end{aligned} \tag{6.63}$$

and, for a given gauge angle ϕ,

$$\begin{aligned} U(\phi) &= \cos\phi I + i\sin\phi N^{11}, \\ V(\phi) &= +i\sin\phi N^{02}. \end{aligned} \tag{6.64}$$

Then the transition densities are

$$\begin{aligned} \rho(\phi) &= +e^{+i\phi}V^*[U^*(\phi)]^{-1}V^T, \\ \kappa^{10}(\phi) &= +e^{+i\phi}V^*[U^*(\phi)]^{-1}U^T, \\ \kappa^{01}(\phi) &= -e^{-i\phi}U^*[U^*(\phi)]^{-1}V^T \end{aligned} \tag{6.65}$$

Bottom line: the total energy $E[\rho,\kappa]$ can be expressed as a functional of the transition densities alone, which can be expressed functions of the U and the V matrices.

Caveats

- PAV: if pairing has disappeared during HFB iterations, PAV won't change a thing
- VAP: very costly to implemented
- PAV/VAP: not viable if EDF not strictly derived from the expectation value of a *density-independent* pseudopotential on the HFB vacuum.

6.5 Exercise

Exercise 16.

Starting from a two-body Hamiltonian, calculate the energy on the Bogoliubov vacuum as a functional of ρ, κ and κ^*.

Exercise 17.

Derive the HFB equation by applying the variational principle: the energy should be a minimum with respect to variations of the generalized density, under the condition that said generalized density is a projector.

Exercise 18.

Using the canonical basis, show that a fully paired vacuum always correspond to a superposition of eigenstates of $\hat{N}$ with even number of particles, and that the prescription (6.56) gives a superposition of odd-particle eigenstates.

Exercise 19.

Show that the BCS ansatz for the wavefunction derives from the form of the HFB vacuum and the Bloch-Messiah theorem

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Exercise 20.

Prove that the BCS wave function is not an eigenstate of the particle number operator

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Lecture 7

Random Phase Approximation [Week 2, day 2]

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7.1 Nuclear vibrations

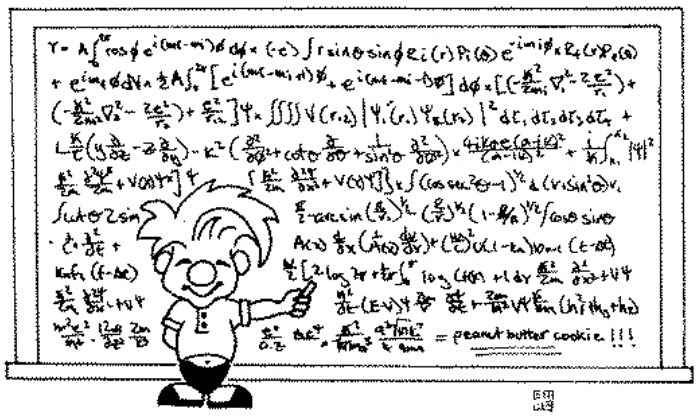

Figure 7.1: today's lecture

Exploring nuclear excitations.

- 1947 Baldwin-Klaiber observe a giant dipole resonance (GDR) in photo-nuclear reactions
- 1972 giant quadrupole resonance
- 1977 giant dipole resonance

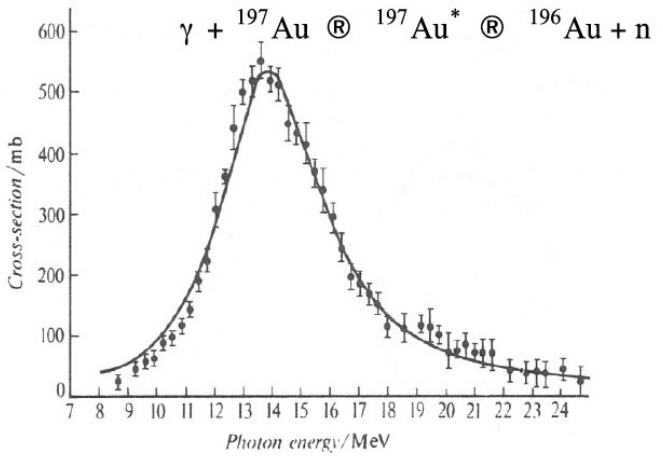

Figure 7.2: Giant resonance of photo disintegration in ^{197}Au. The yield of neutrons is shown as a function of the energy of the monochromatic photons used to produce the reaction.

Let's consider an electromagnetic process. The electric multipole moment associated with an electromagnetic transition E_λ can be expressed as [9]

$$M(E\lambda;\mu) = \frac{(2\lambda+1)!!}{q^\lambda(\lambda+1)} \int d^3r \left\{ \rho Y_{\lambda\mu} \frac{d}{dr} r j_\lambda(qr) + i\frac{q}{c}\mathbf{j}\cdot\mathbf{r} Y_{\lambda\mu} j_\lambda(qr) \right\} \tag{7.1}$$

where q is the momentum transfer, $j_\lambda(qr)$ is the spherical Bessel function, ρ is the charge density and $\mathbf{j}$ is the current density.

For a photon of 10 MeV the exchange momentum is $q - 0.25$ fm $^{-1}$ thus $qr << 1$. We can make an expansion of the Bessel function as

$$j_\lambda(qr) \approx \frac{(qr)^\lambda}{(2\lambda+1)!!}\left[1 - \frac{1}{2}\frac{(qr)^2}{2\lambda+3} + \dots\right] \tag{7.2}$$

we replace in previous equation and we stop at first order. We get

$$M(E\lambda;\mu) = \frac{(2\lambda+1)!!}{q^\lambda(\lambda+1)} \int d^3r \left\{ \rho Y_{\lambda\mu} \frac{d}{dr}\left(\frac{(qr)^\lambda}{(2\lambda+1)!!}\right)\right\} \tag{7.3}$$

$$= \int \rho r^\lambda Y_{\lambda\mu} d^3r \tag{7.4}$$

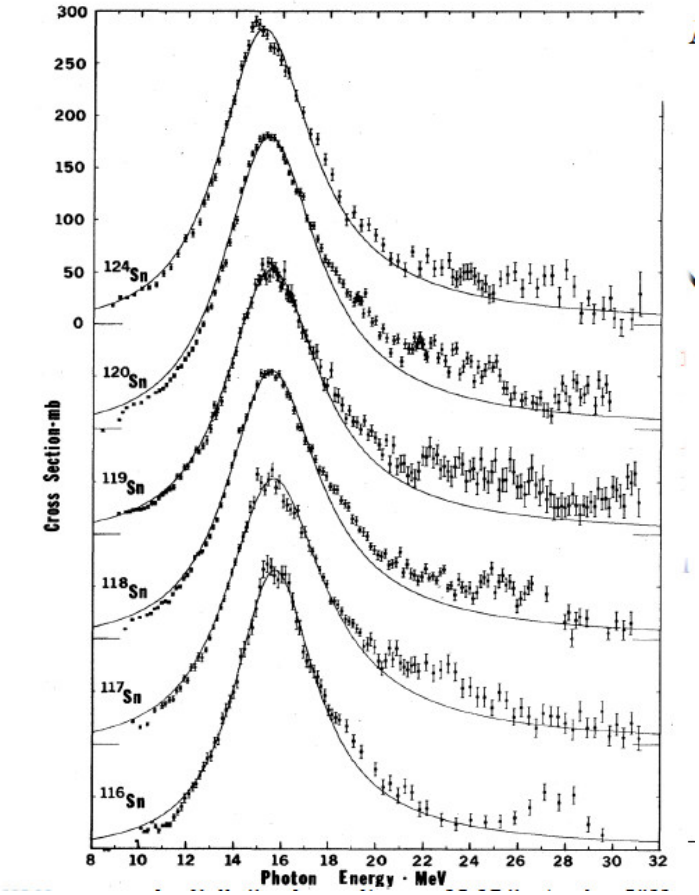

Figure 7.3: Giant resonance dipole resonance with mono energetic photons in Sn isotopes

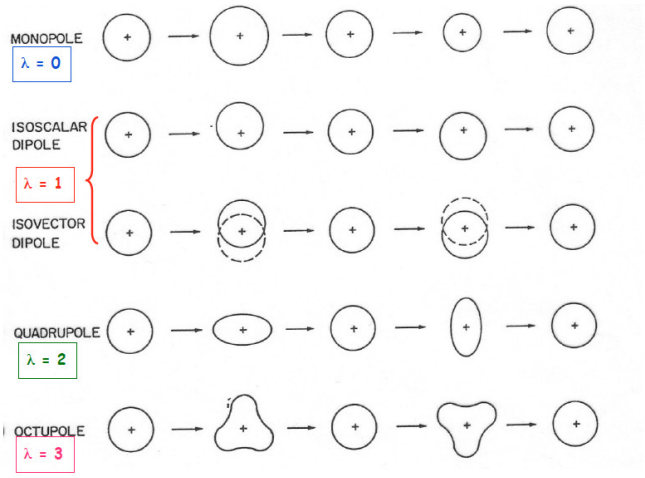

Figure 7.4: Schematic representation of collective natural parity modes.

by assuming that the charge density is written as

	$\Delta S=0$ $\Delta T=0$	$\Delta S=0$ $\Delta T=1$	$\Delta S=1$ $\Delta T=0$	$\Delta S=1$ $\Delta T=1$
L=0		$\sum \tau_i$ IAS		$\sum \sigma_i\tau_i$ GTR
	$\sum_i r_i^2$ ISGMR	$\sum r_i^2\tau_i$ IVGMR	$\sum r_i^2\sigma_i$ ISSMR	$\sum r_i^2\sigma_i\tau_i$ IVSMR
L=1		$\sum r_i Y_m^1\tau_i$ IVGDR	$\sum r_i Y_m^1\sigma_i$ ISSDR	$\sum r_i Y_m^1\sigma_i\tau_i$ IVSDR
	$\sum r_i^3 Y_m^1$ ISGDR			
L=2	$\sum r_i^2 Y_m^2$ ISGQR	$\sum r_i^2 Y_m^2\tau_i$ IVGQR	$\sum r_i^2 Y_m^2\sigma_i$ ISSQR	$\sum r_i^2 Y_m^2\sigma_i\tau_i$ IVSQR
L=3	$\sum r_i^3 Y_m^2$ ISGOR	$\sum r_i^3 Y_m^2\tau_i$ IVGOR	$\sum r_i^3 Y_m^2\sigma_i$ ISSOR	$\sum r_i^3 Y_m^2\sigma_i\tau_i$ IVSOR

Table 7.1: Summary of probes used to excited collective states

$$\rho(r) = \sum_k e\left(\frac{1}{2} - t_{zk}\right)\delta(\mathbf{r} - \mathbf{r}_k) \tag{7.5}$$

where we neglect relativistic effects and assuming point like particles. We can substitute and we get

$$M(E\lambda;\mu) \quad = \quad \sum_k e\left(\frac{1}{2} - t_{zk}\right) r_k^\lambda Y_{\lambda\mu}(\Omega_k) \tag{7.6}$$

the first term does not depend on isospin and thus it probes *isoscalar* modes, the second probes *isovector* modes. In this expansion a word of caution for monopole modes. In this case $\lambda = 0$ our approximation does not work and so we have to go up to a second order in the expansion so

$$M(E_0) = \frac{1}{4} r \sum_k r_k^2 - \frac{1}{2} e \sum_k t_{zk} r_k^2 \tag{7.7}$$

In Tab.7.1 we summarise the possible probes used to excited various collective states. We distinguish between isospin flip or not ($\Delta T = 0, 1$) and non spin-flip or spin-flip ($\Delta S = 0, 1$).

Since most of the time the residual interaction is diagonal in isospin, we can separate out the calculation for charge exchange process and charge conserving ones.

7.1.1 Linear response theory

We assume that an external time dependent field perturbs our HF ground state.

$$F(t) = Fe^{-i\omega t} + F^\dagger e^{i\omega t} \tag{7.8}$$

we assume that F is one body operator $F(t) = \sum_{kl} f_{kl} a_k^\dagger a_l$. the field is weak so that we can assume only small variations around the ground state.

The density matrix is now time-dependent and reads

$$\rho(t)_{kj} = \langle \Phi(t) | a_l^\dagger a_k | \Phi(t) \rangle \tag{7.9}$$

We assume that at *any* time $\rho(t)$ corresponds to a Slater determinant $\rho^2 = \rho /$ So the density obeys the equation of motion

$$i\hbar \frac{d\rho}{dt} = [h[\rho] + f(t), \rho] \tag{7.10}$$

this is the Time Dependent Hartree Fock (TDHF) equation obtained by time derivative of the density matrix.

Working in the small amplitude limit we can expand the density around the g.s. value $\rho^{(0)}$ as

$$\begin{aligned} \rho(t) &= \rho^{(0)} + \delta\rho(t) & (7.11)\\ &= \rho^{(0)} + \rho^{(1)} e^{-i\omega t} + \rho^{(1)\dagger} e^{i\omega t} & (7.12) \end{aligned}$$

We work for convenience in the HF basis of the ground state density $\rho^{(0)}$. In this case the density is diagonal and we have 1 and 0 occupation number.

$$\begin{aligned} i\hbar \frac{d\rho}{dt} &= [h[\rho] + f(t), \rho] & (7.13)\\ &= \left[h[\rho^{(0)} + \delta\rho(t)] + f(t), \rho^{(0)} + \delta\rho(t) \right] & (7.14)\\ &= \left[h[\rho^{(0)}] + \frac{\delta h}{\delta \rho} \delta\rho(t) + f(t), \rho^{(0)} + \delta\rho(t) \right] & (7.15) \end{aligned}$$

we expand up to linear order. We observe that in HF basis

$$\rho^{(0)}_{\mu\nu} = \delta_{\mu\nu} \rho^{(0)}_\mu \begin{cases} 0 & \text{particle} \\ 1 & \text{hole} \end{cases} \tag{7.16}$$

$$h^0_{\mu\nu} = h[\rho^0]_{\mu\nu} = \delta_{\mu\nu} \varepsilon_\mu \tag{7.17}$$

$$\rho^2 = \rho \to \rho^0 \delta\rho + \delta\rho\rho^0 = \delta\rho \tag{7.18}$$

We observe that the only non vanishing matrix elements of ρ^1 are the ph hp excitations. We get

$$i\hbar \frac{d\rho}{dt} = [h_0, \delta\rho] + [f, \rho^{(0)}] + \left[\frac{\delta h}{\delta \rho} \delta\rho, \rho^{(0)} \right] \tag{7.19}$$

$$\frac{\delta h}{\delta \rho}\delta\rho = \sum_{im}\left(\left.\frac{\delta h}{\delta \rho_{mi}}\right|_{\rho=\rho^{(0)}}\delta\rho_{mi} + \left.\frac{\delta h}{\delta \rho_{im}}\right|_{\rho=\rho^{(0)}}\delta\rho_{im}\right) \tag{7.20}$$

in this equation all particle-particle and hole-hole matrix elements vanish and we have as possible excitations only particle-hole or hole-particle.

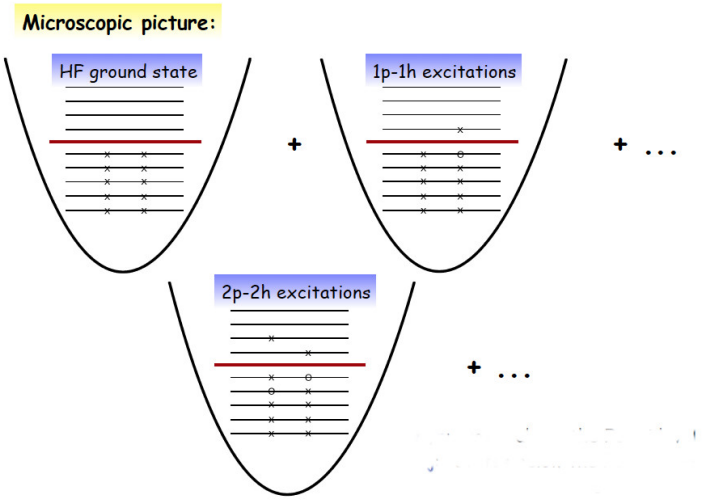

Figure 7.5: Schematic representation of excited states in nuclei.

These equations can be expressed in a more elegant matrix form

$$\left\{\begin{pmatrix} A & B \\ B^* & A^* \end{pmatrix} - \hbar\omega \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}\right\}\begin{pmatrix} \rho^{(1)}_{ph} \\ \rho^{(1)}_{hp} \end{pmatrix} = \begin{pmatrix} f_{ph} \\ f_{hp} \end{pmatrix} \tag{7.21}$$

we have defined

$$A_{minj} = (\varepsilon_m - \varepsilon_i)\delta_{ij}\delta_{mn} + \frac{\partial h_{mi}}{\partial \rho_{nj}} \tag{7.22}$$

$$B_{minj} = \frac{\partial h_{mi}}{\partial \rho_{jn}} \tag{7.23}$$

This is called linear response since there is a linear relation between ρ^1 and the external field f.

Remember that

$$\bar{v}_{psqr} = \frac{\partial h_{pq}}{\partial \rho_{rs}} = \frac{\partial^2 E[\rho]}{\partial \rho_{qp}\partial \rho_{rs}} \tag{7.24}$$

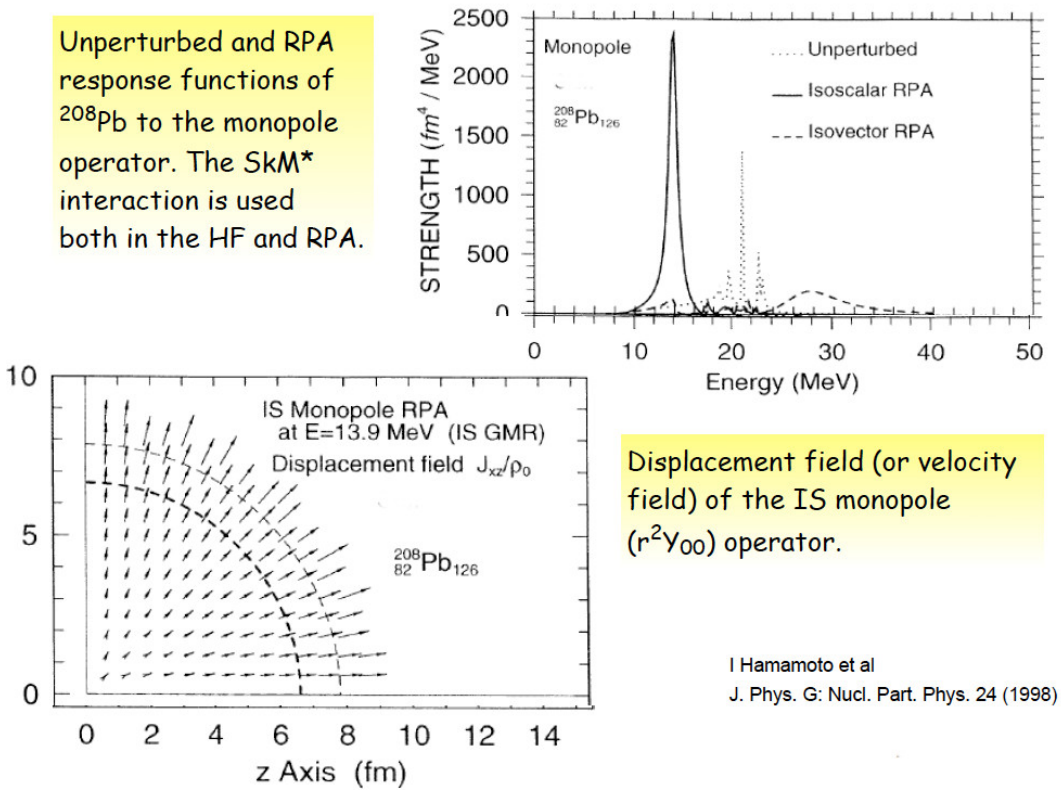

Figure 7.6: Giant monopole excitation in ^{208}Pb.

The RPA approximation is the small amplitude limit of the TDHF.

Within the RPA approximation one can calculate the excited states as

$$Q^\dagger_\nu = \sum_{mi} X^\nu_{mi} a^\dagger_m a_i - \sum_{mi} Y^\nu_{mi} a^\dagger_i a_m \tag{7.25}$$

This operator creates the excited states so that $Q_\nu |RPA\rangle = 0$

We have to impose orthogonalisation relations

$$\langle \nu | \nu' \rangle = \delta_{\nu\nu'} = \langle RPA | [Q_\nu, Q^\dagger_{\nu'}] | RPA \rangle \approx \langle HF | [Q_\nu, Q^\dagger_{\nu'}] | HF \rangle \tag{7.26}$$

so we get

$$\delta_{\nu\nu'} = \sum_{mi} \left(X^{\nu *}_{mi} X^{\nu'}_{mi} - Y^{\nu *}_{mi} Y^{\nu'}_{mi} \right) \tag{7.27}$$

when $|RPA\rangle \approx |HF\rangle$ we use the *quasi-boson* approximation the X, Y are intrpeted as the probability of finding the state $a^\dagger_m a_i |0\rangle$ and $a^\dagger_i a_m |0\rangle$ in the exctied state $|\nu\rangle$.

A possible extension of RPA is second-RPA; e can consider not only 1p-1h excitations but also 2p-2h

$$Q^\dagger_\nu = \sum_{ph} X^\nu_{ph} a^\dagger_p a_h - Y^\nu_{hp} a^\dagger_h a_p \tag{7.28}$$

$$+ \sum_{p<p';h<h'} X^\nu_{php'h'} a^\dagger_p a_h a^\dagger_{p'} a_{h'} - Y^\nu_{php'h'} a^\dagger_h a_p a^\dagger_{h'} a_{p'} \tag{7.29}$$

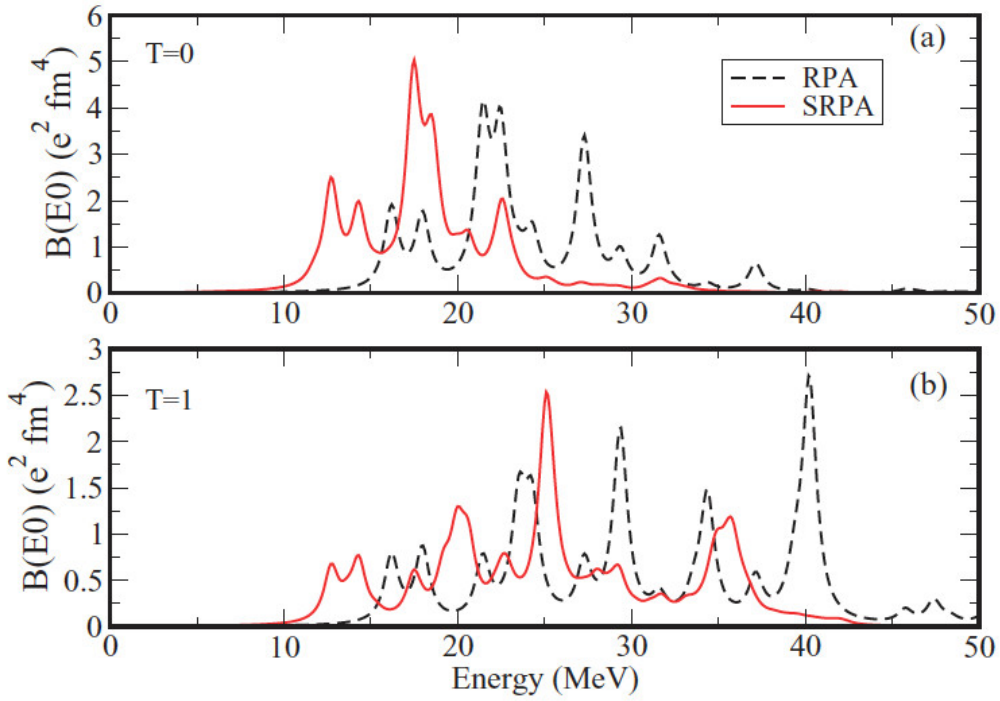

FIG. 3. (Color online) RPA [dashed (black) lines] and SRPA [full (red) lines] for the isoscalar (upper panel) and isovector (lower panel) monopole strength distributions.

Figure 7.7: (ct. Gamabcurta et al. PRC81 (2010)

7.2 Sum rules

The sum rule is an important property of the calculation since it can be related to important properties of the response function.

The sum rule of an operator $F = \sum f_{pq} a^\dagger_p a_q$ is defined as

$$S_k = \sum_\nu (E_\nu - E_0)^k |\langle \nu | F | 0 \rangle|^2 \tag{7.30}$$

The $|\nu\rangle$ represents the complete set of the eigenstates of the exact hamiltonian H with energies E_ν. The most important sum rule is the S_1 also called Energy Weighted Sum Rule (EWSR). In this case one can show that

$$S_1 = \sum_\nu (E_\nu - E_0)|\langle\nu|F|0\rangle|^2 \tag{7.31}$$

To prove this we consider an operator $\hat{C} = [\hat{H}, \hat{F}]$ which is hermitian

We now calculate

$$\begin{aligned}
\langle 0|[F,C]|0\rangle &= \langle 0|FC|0\rangle - \langle 0|CF|0\rangle & (7.32)\\
&= \sum_\nu \langle 0|F|\nu\rangle\langle\nu|C|0\rangle - \langle 0|C|\nu\rangle\langle\nu|F|0\rangle & (7.33)\\
&= \sum_\nu \langle 0|F|\nu\rangle\langle\nu|F|0\rangle(E_\nu - E_0) - (E_0 - E_\nu)\langle 0|F|\nu\rangle\langle\nu|F|0\rangle & (7.34)\\
&= 2\sum_\nu (E_\nu - E_0)\langle\nu|F|0\rangle^2 & (7.35)
\end{aligned}$$

In the RPA case the ground state $|0\rangle$ is approximated by the $|HF\rangle$ ground state. We assume that our excitation operator gives

$$\langle 0|F|0\rangle = 0 \tag{7.36}$$

We consider a simple Hamiltonian $H = T+V$ and an operator of the form $F = \sum_{i=1}^{A} e r_i^L Y_{LM}(\Omega_i)$

We get for isoscalar probes ($\lambda > 2$)

$$S_1^{IS}(\lambda) = \frac{\hbar^2}{2m}\frac{\lambda(\lambda+1)^2}{4\pi A}\langle r^{2\lambda-2}\rangle \tag{7.37}$$

For isovector probes we define

$$F_{LM} = \frac{eN}{A}\sum_{i=1}^{Z} r^L Y_{LM} - \frac{eZ}{A}\sum_{i=1}^{N} r^L Y_{LM} \tag{7.38}$$

this effective charge factor comes to correct the center of mass correction.

$$S_1^{IV}(\lambda) = \frac{\hbar^2}{2m}\frac{\lambda(\lambda+1)^2}{4\pi}\left\{\frac{N^2 Z}{A^2}\langle r^{2\lambda-2}\rangle_p + \frac{NZ^2}{A^2}\langle r^{2\lambda-2}\rangle_n\right\} \tag{7.39}$$

Notice that for J=0 and J=1 there are some differences in the operators. See references.

Very often the properties of the nucleus relevant to experiment can be related to weighted integrals of the strength function

$$I_f = \int f(E)S(E)dE \tag{7.40}$$

the expression of f is supposed to be know. This function depends on the physical properties and not on the nuclear structure properties. We assume it continuos, but it could not be the case. We can expand the weighted function

$$f(E) = \sum_k \frac{1}{k!} f^k(\bar{E})(E-\bar{E})^k \tag{7.41}$$

$$\begin{aligned} I_f &= f(\bar{E})m_0 + f'(\bar{E})(m_1 - \bar{E}m_0) + \dots & (7.42)\\ &= \sum_k \frac{1}{k!} f^k(\bar{E}) \sum_{i=0}^{k} \left(\begin{array}{c} k \\ i \end{array} \right) (-)^i m_{k-i} \bar{E}^i & (7.43) \end{aligned}$$

knowing all positive moment we get complete information on the strength function!!

7.2.1 Practical example: separable interaction

We take a simple separable 2-body interaction that we can write as

$$V = -\chi \sum_{ij}^{N} Q(i)Q(j) \tag{7.44}$$

so that the matrix elements can be written as[1] and we take only ph excitations (Tam Dancoff approximations)

$$\langle v \rangle_{mjin} \approx -\chi \langle m|Q|i\rangle \langle n|Q|j\rangle \tag{7.45}$$

So replacing in the TD equation (we stay in 1 D system for simplicity)

$$(\varepsilon_{mi} - E)Y_{mi} = \chi Q_{mi} \sum_{nj}^{*} Y_{nj} \tag{7.46}$$

[1] no exchange!

We define $N = \chi Q_{mi} \sum^*_{nj} Y_{nj}$ and we replace in Eq.7.46. We get

$$Y_{mi} = \frac{NQ_{mi}}{\varepsilon_{mi} - E} \tag{7.47}$$

$$N = \chi Q_{mi} \sum_{nj}^{*} Y_{nj} \tag{7.48}$$

$$N = \chi N \sum_{nj} \frac{Q^2_{mi}}{\varepsilon_{mi} - E} \tag{7.49}$$

or more simplify

$$\frac{1}{\chi} = \sum_{nj} \frac{Q^2_{mi}}{\varepsilon_{mi} - E} \tag{7.50}$$

this can be solved graphically. In Fig.7.8 we show a schematic representation of a possible solution for Eq..7.50.

From this figure we observe that according to the sign of χ ,i.e. the residual interaction we have a low-lying state or not.

See for example the position of lowest 2^+ in nuclei!! Also for small residual interactions we obtain a collective excitations which is obtained by superpositions of other *ph* states.

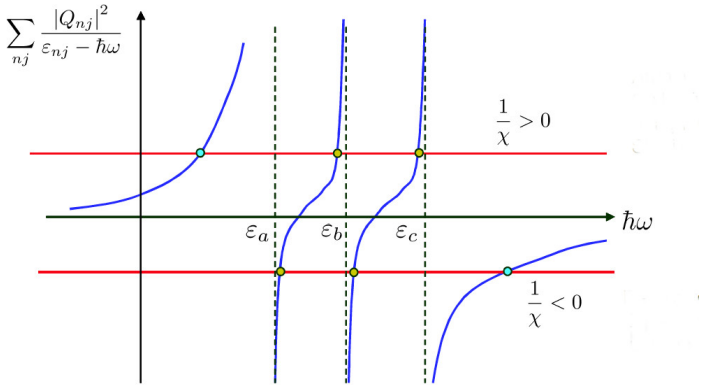

Figure 7.8: Graphical solution of Eq.7.50.

7.2.2 QRPA

The derivation follows exactly the same steps, but instead of ρ we use the $\mathcal{R} = \begin{pmatrix} \rho & \kappa \\ -\kappa^* & 1-\rho^* \end{pmatrix}$

in this case the operator that creates the excitation is

$$Q^\dagger_\nu = \sum_{K\leq K'} X^\nu_{KK'}\alpha^\dagger_K\alpha^\dagger_{K'} - Y^\nu_{KK'}\alpha_{K'}\alpha_K \tag{7.51}$$

The equations look formally the same, the novelty is that now we have both ph excitations and pp and hh.

Let's write down the QRPA equation (just to give you a flavour!) in canonical basis [2]

$$\sum_{L<L'} \begin{pmatrix} A_{KK',LL'} & B_{KK',LL'} \\ -B^*_{KK',LL'} & -A^*_{KK',LL'} \end{pmatrix} \begin{pmatrix} X^k_{LL'} \\ Y^k_{LL'} \end{pmatrix} = E^k \begin{pmatrix} X^k_{KK'} \\ Y^k_{KK'} \end{pmatrix} \tag{7.52}$$

You can find explict expressions of the A, B matrix in Ref [9], the residual interaction now is

$$V^{ph}_{KLK'L'} = \frac{\delta^2 E[\rho,\kappa,\kappa^*]}{\delta\rho_{K'K}\delta\rho_{L'L}} \tag{7.53}$$

$$V^{pp}_{K'KL'L} = \frac{\delta^2 E[\rho,\kappa,\kappa^*]}{\delta\kappa^*_{K'K}\delta\kappa_{L'L}} \tag{7.54}$$

If your functional contains mixed terms as $\kappa\rho$ then you need to take into account mixed derivatives!

$$V^{3p1h}_{K'KL'L} = \frac{\delta^2 E[\rho,\kappa,\kappa^*]}{\delta\kappa_{K'K}\delta\rho_{LL'}} = V^{3p1h*}_{LL'K'K} \tag{7.55}$$

7.2.3 Spurious states

We assume that the hamiltonian H is invariant under a continuos symmetry operation generated by a one-body operator $\hat{P}$ *i.e.* translation, particle number, angular momentum... We assume that the HF(B) solution violates such a symmetry

$$[\rho_0, \hat{P}] \neq 0 \tag{7.56}$$

since ρ_0 is diagonal in HF basis, this means that the non-zero matrix elements of P are the ph. Since the exact hamiltonian commutes with $\hat{P}$

$$[H, \hat{P}] = 0 \tag{7.57}$$

the $\hat{P}$ is an exact solution of the RPA equation. This means

[2] The basis in which the density ρ is diagonal!

$$\begin{pmatrix} A & B \\ B^* & A^* \end{pmatrix} \begin{pmatrix} P \\ -P^* \end{pmatrix} = 0 \tag{7.58}$$

where P is the vector P_{mi} in particle-hole space

$$|P\rangle = \sum_{mi} \left(P_{mi} a_m^\dagger a_i + P_{mi}^* a_i^\dagger a_m \right) |RPA\rangle \tag{7.59}$$

If the calculations are performed exactly, the spurious solution separates out and it is orthonormal to the other phonons.

7.3 Exercise: matrix element in spherical symmetry

7.3.1 Couplings l, s and jj

When coupling two wave functions we can use two schemes: jj or LS. This means[3] In jj scheme we couple spin χ and angular momentum Y_{lm_l}

$$|j_1 j_2 l_1 l_2 JM\rangle = \sum_{m_1 m_2} C^{JM}_{j_1 m_1; j_2 m_2} \sum_{m_l^1 m_s^1} \sum_{m_l^2 m_s^2} C^{j_1 m_1}_{l_1 m_l^1; \frac{1}{2} m_s^1} C^{j_2 m_2}_{l_2 m_l^2; \frac{1}{2} m_s^2} Y_{l_1 m_l^1}(1) \chi_{m_s^1}(1) Y_{l_2 m_l^2}(2) \chi_{m_s^2}(2) \tag{7.60}$$

here $Cj_3 m_3{}_{j_1 m_1 j_2 m_2}$ is the Clebsh-Gordan. If you prefer working in 3j notation[4]

$$Cj_3 m_3{}_{j_1 m_1 j_2 m_2} (-)^{j_1 - j_2 + m_3} \hat{j}_3 \begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & -m_3 \end{pmatrix} \tag{7.61}$$

in the LS coupling we make

7.3.2 Particle-particle and particle-hole matrix element

It is important to separate out the couplings involving particle-particle and particle-hole matrix elements in jj-coupling.

- ${}_J\langle ab^{-1}|V|c^{-1}d\rangle_J$ particle-hole
- ${}_J\langle ad|V|cb\rangle_J$ particle-particle

[3] We neglect radial part since it not essential for the discussion

[4] Remember $\hat{j} = \sqrt{2j+1}$

To go from one to the other we use the so-called Pandya transformation.

$$
\begin{aligned}
{}_J\langle ab^{-1}|V|c^{-1}d\rangle'_J &= \sum_{J'} \hat{J'}^2_{J'} \langle ad|V|bc\rangle_{J'} \sum_{MM'} \sum_{\text{all } m} (-)^{j_b+j_d+m_b+m_d} \\
&\times \begin{pmatrix} j_a & j_b & J \\ m_a & m_b & -M \end{pmatrix} \begin{pmatrix} j_a & j_c & J' \\ m_a & -m_c & -M' \end{pmatrix} \begin{pmatrix} j_d & j_b & J' \\ -m_d & m_b & M' \end{pmatrix} \begin{pmatrix} j_c & j_d & J \\ m_c & m_d & -M \end{pmatrix} \\
&= \sum_{J'} \hat{J'}^2_{J'} \langle ac|V|bd\rangle_{J'} \begin{Bmatrix} j_a & j_b & J \\ j_d & j_c & J' \end{Bmatrix}
\end{aligned} \tag{7.62}
$$

we use the shorthand notation $\hat{j} = \sqrt{2j+1}$. This is know as Pandya transformation and allow us to go from one coupling scheme to the other in a simple way.

Calculate the matrix element of $A\delta(\mathbf{r}-\mathbf{r}')$ on a spherical nucleus characterized by the w.f. ϕ_{nlj}. For simplicity we consider only 1 species, so that we can neglect isospin quantum number. The wave function of the single particle state reads

$$
\phi_{nljm}(r,\Omega) = \frac{u_{nlj}(r)}{r} \sum_{m_l m_s} C^{jm}_{lm_l,\frac{1}{2}m_s} Y_{lm_l}(\Omega)\chi_{\frac{1}{2}m_s} \tag{7.63}
$$

calculate

$$
{}_J\langle ac^{-1}|V|b^{-1}d\rangle_J = \tag{7.64}
$$

$$
{}_J\langle ac|V|bd\rangle_J = \tag{7.65}
$$

for simplicity you can consider only $J = 0$, optionally you can consider the general case ($J \neq 0$)

you have to consider just the direct term (no exchange: if we suppose the residual interaction comes from functional derivative, this is already taken into account at functional level) Use the formula

$$
\delta(\mathbf{r}_1 - \mathbf{r}_2) = \sum_{\lambda\mu} (-)^\lambda \frac{\delta(r_1 - r_2)}{r^2} Y_{\lambda\mu}(1) Y_{\lambda-\mu} \tag{7.66}
$$

Lecture 8

Nuclear collective motion: Configuration mixing [Week 2, day 3]

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8.1 Configuration mixing

8-1: Correlations

Fermion states that are not equal to product states are called correlated states.

Remember that product states form a basis of the many-fermion Hilbert space, so an arbitrary many-fermion wave function $\Psi(x_1, \ldots, x_A)$ can always be represented as a linear combination of product states:

$$\Psi(x_1, \ldots, x_A) = \sum_{\mu_1,\ldots,\mu_A} A_{\mu_1,\ldots,\mu_A} \Phi_{\mu_1,\ldots,\mu_A}(x_1, \ldots, x_A) \tag{8.1}$$

or as a multi-dimensional integral over the product states:

$$|\Psi\rangle = \int \mathrm{d}\tilde{Z}\, f(\tilde{Z}) |\Phi(\tilde{Z})\rangle, \tag{8.2}$$

were $|\Phi(\tilde{Z})\rangle$ are the Thouless product states [generalized coherent states] paramatrized by complex Thouless matrices $\tilde{Z}_{ph}$:

$$|\Phi(\tilde{Z})\rangle \equiv |\tilde{Z}\rangle = \exp\left(\sum_{ph} \tilde{Z}^*_{ph} a^+_p a_h\right) a^+_1 \ldots a^+_A |0\rangle, \tag{8.3}$$

for which the unity resolution holds:

$$\hat{I} = \int w(\tilde{Z}) \mathrm{d}\tilde{Z} |\tilde{Z}\rangle\langle\tilde{Z}|, \tag{8.4}$$

$$\begin{aligned} w(\tilde{Z}) &= W\langle\tilde{Z}|\tilde{Z}\rangle^{-M+1} = W \det(1+\tilde{Z}\tilde{Z}^+)^{-M+1}, & \text{(8.5a)} \\ W &= \pi^{A(A-M)} \prod_{\nu=1}^{M-A} \frac{(\nu+A)!}{\nu!}, & \text{(8.5b)} \\ d\tilde{Z} &= \prod_{ph} d\Re(\tilde{Z}_{ph}) d\Im(\tilde{Z}_{ph}). & \text{(8.5c)} \end{aligned}$$

Representations (8.1) and (8.2) motivate introducing the following *approximate* models:

- The shell model (SM) or no-core shell model (NCSM):

$$\Psi(x_1, \ldots, x_A) \simeq \sum_{\mu_1,\ldots,\mu_{A'}} A_{\mu_1,\ldots,\mu_{A'}} \Phi_{\mu_1,\ldots,\mu_{A'}}(x_1, \ldots, x_{A'}) \otimes |\mathrm{core}\rangle \tag{8.6}$$

  for A' valence particles occupying M single-particle states ϕ_μ for $\mu = 1, \ldots, M$.

- The configuration interaction (CI) models:

$$\Psi(x_1, \ldots, x_A) \simeq \sum_k A_k \Phi_k(x_1, \ldots, x_A) \tag{8.7}$$

  for $\Phi_k(x_1, \ldots, x_A)$ belonging to an **appropriately selected** discrete set of product states of A particles.

- The generator coordinate method (GCM) models:

$$\Psi(x_1, \ldots, x_A) \simeq \int \mathrm{d}q\, f(q) \Phi_q(x_1, \ldots, x_A), \tag{8.8}$$

  for $|\Phi(q)\rangle = |\Phi(\tilde{Z}(q))\rangle$ constituting an **appropriately selected** continuous family of product states of A particles.

8-2: Generator coordinate method

Postulates an approximation of the many-fermion state by the integral:

$$|\Psi\rangle = \int \mathrm{d}q\, f(q) |\Phi(q)\rangle, \tag{8.9}$$

where $|\Phi(q)\rangle = |\Phi(\tilde{Z}[q])\rangle$ denotes a family of product states (generator states) parametrized by the generator coordinate(s) q.

8.2 The Hill-Wheeler equation

$$\langle\Psi|\hat{H}|\Psi\rangle = \int \mathrm{d}q\mathrm{d}q'\, f^*(q)\mathcal{H}(q,q')f(q'), \tag{8.10a}$$

$$\langle\Psi|\Psi\rangle = \int \mathrm{d}q\mathrm{d}q'\, f^*(q)\mathcal{I}(q,q')f(q') = 1, \tag{8.10b}$$

where

$$\mathcal{H}(q,q') = \langle\Phi(q)|\hat{H}|\Phi(q')\rangle, \tag{8.11a}$$

$$\mathcal{I}(q,q') = \langle\Phi(q)|\Phi(q')\rangle, \tag{8.11b}$$

and,

$$\mathcal{H}(q,q') = \mathcal{H}^*(q',q), \tag{8.12a}$$

$$\mathcal{I}(q,q') = \mathcal{I}^*(q',q), \tag{8.12b}$$

for

$$\langle\Phi(q)|\Phi(q)\rangle = 1, \tag{8.13}$$

The average energy:

$$E = \frac{\langle\Psi|\hat{H}|\Psi\rangle}{\langle\Psi|\Psi\rangle} \tag{8.14}$$

is a functional of the weight function $f(q)$, E=$E[f]$. By varying the average energy with respect to the weight function we obtain [17]:

8-3: The Hill-Wheeler equation

$$\boxed{\int \mathrm{d}q'\Big[\mathcal{H}(q,q') - E\mathcal{I}(q,q')\Big]f(q') = 0.} \tag{8.15}$$

A discretization corresponds to a CI model:

$$\sum_j \mathcal{H}_{ij}f_j = E\sum_j \mathcal{I}_{ij}f_j, \tag{8.16}$$

where $\mathcal{H}_{ij} \equiv \mathcal{H}(q_i,q_j)$, $\mathcal{I}_{ij} \equiv \mathcal{I}(q_i,q_j)$, and $f_j \equiv f(q_j)$.

The square-root kernel $\mathcal{I}^{1/2}(q,q')$:

$$\mathcal{I}(q,q') = \int \mathrm{d}q''\, \mathcal{I}^{1/2}(q,q'')\,\mathcal{I}^{1/2}(q'',q'). \tag{8.17}$$

allows us to define for each kernel $\mathcal{O}(q,q')$ its reduced kernel $\tilde{\mathcal{O}}(q,q')$:

$$\mathcal{O}(q,q') = \int \mathrm{d}q''\mathrm{d}q'''\, \mathcal{I}^{1/2}(q,q'')\,\tilde{\mathcal{O}}(q'',q''')\,\mathcal{I}^{1/2}(q''',q'), \tag{8.18}$$

which gives:

8-4: Integral GCM Schrödinger equation

$$\boxed{\int \mathrm{d}q'\,\tilde{\mathcal{H}}(q,q')\,g(q') = E\,g(q),} \tag{8.19}$$

where

$$g(q) = \int \mathrm{d}q'\,\mathcal{I}^{1/2}(q,q')\,f(q'), \tag{8.20}$$

and

$$\int \mathrm{d}q\,|g(q)|^2 = 1, \tag{8.21}$$

The inverse square-root kernel:

$$\int \mathrm{d}q''\,\mathcal{I}^{-1/2}(q,q'')\,\mathcal{I}^{1/2}(q'',q') = \delta(q-q'). \tag{8.22}$$

does not exist! Let us check the spectrum of the norm kernel:

$$\int \mathrm{d}q'\,\mathcal{I}(q,q')\,i_k(q') = n_k\,i_k(q). \tag{8.23}$$

which gives orthogonal *natural* states

$$\int \mathrm{d}q\,i_k^*(q)\,i_{k'}(q) = \delta_{kk'}. \tag{8.24}$$

The cut-off expansion:

$$\mathcal{I}(q,q') \simeq \sum_{n_k>n_{\mathrm{cut}}} i_k(q)\,n_k\,i_k^*(q'), \tag{8.25}$$

gives

$$\mathcal{I}^{1/2}(q,q') \simeq \sum_{n_k>n_{\mathrm{cut}}} i_k(q)\,n_k^{1/2}\,i_k^*(q'), \tag{8.26a}$$

$$\mathcal{I}^{-1/2}(q,q') \simeq \sum_{n_k>n_{\mathrm{cut}}} i_k(q)\,n_k^{-1/2}\,i_k^*(q'), \tag{8.26b}$$

and the reduced kernels

$$\tilde{\mathcal{O}}(q,q') \simeq \sum_{\substack{n_k>n_{\mathrm{cut}}\\ n_{k'}>n_{\mathrm{cut}}}} i_k(q)\,\tilde{\mathcal{O}}_{kk'}\,i_{k'}^*(q'), \tag{8.27}$$

where

$$\tilde{\mathcal{O}}_{kk'} = n_k^{-1/2} n_{k'}^{-1/2} \int \mathrm{d}q\mathrm{d}q'\,i_k^*(q)\,\mathcal{O}(q,q')\,i_{k'}(q'). \tag{8.28}$$

and

$$\sum_{k'} \tilde{\mathcal{H}}_{kk'} g_{k'} = E g_k, \tag{8.29}$$

$$g(q) = \sum_k g_k \, i_k(q). \tag{8.30}$$

$$\langle \Psi | \hat{O} | \Psi \rangle = \sum_{kk'} g_k^* \, \tilde{\mathcal{O}}_{kk'} \, g_{k'}. \tag{8.31}$$

8-5: Differential GCM Schrödinger equation

$$\hat{\mathcal{H}}(q) g(q) = E g(q) \tag{8.32}$$

for

$$\mathcal{O}(q,q') = \int \mathrm{d}q'' \, \mathcal{I}^{1/2}(q,q'') \, \hat{\mathcal{O}}(q'') \, \mathcal{I}^{1/2}(q'',q'), \tag{8.33}$$

where $\hat{\mathcal{O}}(q)$ is a differential operator in q.

8.3 Gaussian overlap approximation (GOA)

8-6: Gaussian overlap approximation

Gaussian overlap approximation postulates the approximation of the norm and Hamiltonian kernels by the Gauss functions:

$$\mathcal{H}_G(q,q') = \mathcal{I}_G(q,q') \Big[h_0(Q) - \tfrac{1}{2} h_2(Q) (q-q')^2 \Big], \tag{8.34a}$$

$$\mathcal{I}_G(q,q') = \exp\left\{ -\tfrac{1}{2} a^2(Q) (q-q')^2 \right\}, \tag{8.34b}$$

where functions $a(Q)$, $h_0(Q)$ i $h_2(Q)$ depend on $Q{=}\frac{1}{2}(q+q')$.

In the GOA we have:

$$\frac{\mathcal{H}(q,q')}{\mathcal{I}(q,q')} \equiv h(q,q') \simeq h_0(Q) - \tfrac{1}{2} h_2(Q) (q-q')^2 + \ldots, \tag{8.35a}$$

$$\log \mathcal{I}(q,q') \equiv i(q,q') \simeq -\tfrac{1}{2} a^2(Q) (q-q')^2 + \ldots, \tag{8.35b}$$

which gives

$$h_0(q) = h(q,q), \tag{8.36a}$$

$$h_2(q) = \left[-\frac{\partial^2 h(q,q')}{\partial (q-q')^2} \right]_{q'=q} = \frac{1}{2} \left[\frac{\partial^2 h(q,q')}{\partial q \partial q'} - \frac{\partial^2 h(q,q')}{\partial q^2} \right]_{q'=q}, \tag{8.36b}$$

$$a^2(q) = \left[-\frac{\partial^2 i(q,q')}{\partial (q-q')^2} \right]_{q'=q} = \frac{1}{2} \left[\frac{\partial^2 i(q,q')}{\partial q \partial q'} - \frac{\partial^2 i(q,q')}{\partial q^2} \right]_{q'=q}. \tag{8.36c}$$

or

$$a(q) = \frac{1}{2}\left[\frac{\partial\tilde{i}(q,q')}{\partial q} - \frac{\partial\tilde{i}(q,q')}{\partial q'}\right]_{q'=q} \tag{8.37}$$

for

$$\tilde{i}(q,q') = \sqrt{-2\log\mathcal{I}(q,q')}. \tag{8.38}$$

Canonical variable:

$$x(q) = \int_{q_0}^{q} \mathrm{d}q'\, a(q'). \tag{8.39}$$

gives

8-7: Gaussian overlap approximation in the canonical variable

$$\begin{aligned} \mathcal{H}_G(x,x') &= \mathcal{I}_G(x,x')\Big[h_0(X) - \tfrac{1}{2}h_2(X)(x-x')^2\Big], && \text{(8.40a)} \\ \mathcal{I}_G(x,x') &= \exp\left\{-\tfrac{1}{2}(x-x')^2\right\}, && \text{(8.40b)} \end{aligned}$$

where functions $a(X)$, $h_0(X)$ i $h_2(X)$ depend on $X{=}\frac{1}{2}(x+x')$.

We can now determine the square-root norm kernel $\mathcal{I}_G^{1/2}(x,x')$ (8.17),

$$\mathcal{I}_G^{1/2}(x,x') = (2/\pi)^{1/4}\exp\left\{-(x-x')^2\right\}, \tag{8.41}$$

and its spectrum (8.23),

$$\begin{aligned} n_k &= (2\pi)^{1/2}\exp\left\{-\tfrac{1}{2}k^2\right\}, && \text{(8.42a)} \\ i_k(x) &= \exp\{ikx\}, && \text{(8.42b)} \end{aligned}$$

see exercise 2.

We can now prove (exercise 3) that

$$\hat{\mathcal{H}} = -\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}x}B(x)\frac{\mathrm{d}}{\mathrm{d}x} + V(x), \tag{8.43}$$

exactly fulfils (8.33) provided the collective mass function $B(x)$ and collective potential $V(x)$ fulfill Fredholm integral equations of the first kind:

$$\begin{aligned} h_0(x) &= (2/\pi)^{1/2}\int \mathrm{d}x'\left[2(x-x')^2B(x') + V(x')\right]\exp\left\{-2(x-x')^2\right\}, && \text{(8.44a)} \\ h_2(x) &= (2/\pi)^{1/2}\int \mathrm{d}x'\, B(x')\exp\left\{-2(x-x')^2\right\}. && \text{(8.44b)} \end{aligned}$$

which can be formally solved through the Fourier transforms:

$$\begin{aligned} V(x) &= (1/2\pi)\int \mathrm{d}k\left[h_0(k) - \tfrac{1}{8}(4-k^2)h_2(k)\right]\exp\left\{k^2/8 - ikx\right\}, && \text{(8.45a)} \\ B(x) &= (1/2\pi)\int \mathrm{d}k\, h_2(k)\exp\left\{k^2/8 - ikx\right\}, && \text{(8.45b)} \end{aligned}$$

where

$$h_j(k) = \int \mathrm{d}x\, h_j(x) \exp\{ikx\}\,. \tag{8.46}$$

If we expand $V(x')$ and $B(x')$ around x,

$$\begin{aligned} V(x') &= V(x) + (x'-x)V'(x) + \tfrac{1}{2}(x'-x)^2 V''(x) + \ldots, & (8.47a)\\ B(x') &= B(x) + (x'-x)B'(x) + \tfrac{1}{2}(x'-x)^2 B''(x) + \ldots, & (8.47b) \end{aligned}$$

than

$$\begin{aligned} V(x) &= h_0(x) - \tfrac{1}{2}h_2(x) - \tfrac{1}{8}V''(x) - \tfrac{1}{8}B''(x), & (8.48a)\\ B(x) &= h_2(x) - \tfrac{1}{8}B''(x). & (8.48b) \end{aligned}$$

or

$$\begin{aligned} V(x) &= h_0(x) - \tfrac{1}{2}h_2(x) - \tfrac{1}{8}h_0''(x) - \tfrac{1}{16}h_2''(x), & (8.49a)\\ B(x) &= h_2(x) - \tfrac{1}{8}h_2''(x). & (8.49b) \end{aligned}$$

In case when the scale a is constant we have:

$$\hat{\mathcal{H}} = -\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}q}B(q)\frac{\mathrm{d}}{\mathrm{d}q} + V(q), \tag{8.50}$$

$$\begin{aligned} h_0(q) &= (2a/\pi)^{1/2} \int \mathrm{d}q' \left[2(q-q')^2 a^4 B(q') + V(q')\right] \exp\left\{-2a^2(q-q')^2\right\}, & (8.51a)\\ h_2(q) &= (2a/\pi)^{1/2} \int \mathrm{d}q'\, B(q') a^4 \exp\left\{-2a^2(q-q')^2\right\}. & (8.51b) \end{aligned}$$

and thus in the lowest order:

$$\begin{aligned} V(q) &= h_0(q) - \tfrac{1}{2}h_2(q)/a^2, & (8.52a)\\ B(q) &= h_2(q)/a^4. & (8.52b) \end{aligned}$$

8.4 Symmetry restoration

8.5 Take-away messages

8.6 Exercises

1. Estimate the dependence of the norm kernel (8.11b) on a difference between the product states.

2. For the Gaussian kernel (8.40b) calculate the its square-root kernel (8.17) and its spectrum and eigen functions (8.23).

3. Prove that the second-order differential operator (8.43) fulfills (8.33) for $B(x)$ and $V(x)$ defined in (8.44).

$$\begin{aligned} (x''-x)^2 + (x''-x')^2 &= 2\left(x'' - \tfrac{1}{2}(x+x')\right)^2 + \tfrac{1}{2}(x-x')^2, & (8.53)\\ 2(x''-x)(x''-x') &= 2\left(x'' - \tfrac{1}{2}(x+x')\right)^2 - \tfrac{1}{2}(x-x')^2. & (8.54) \end{aligned}$$

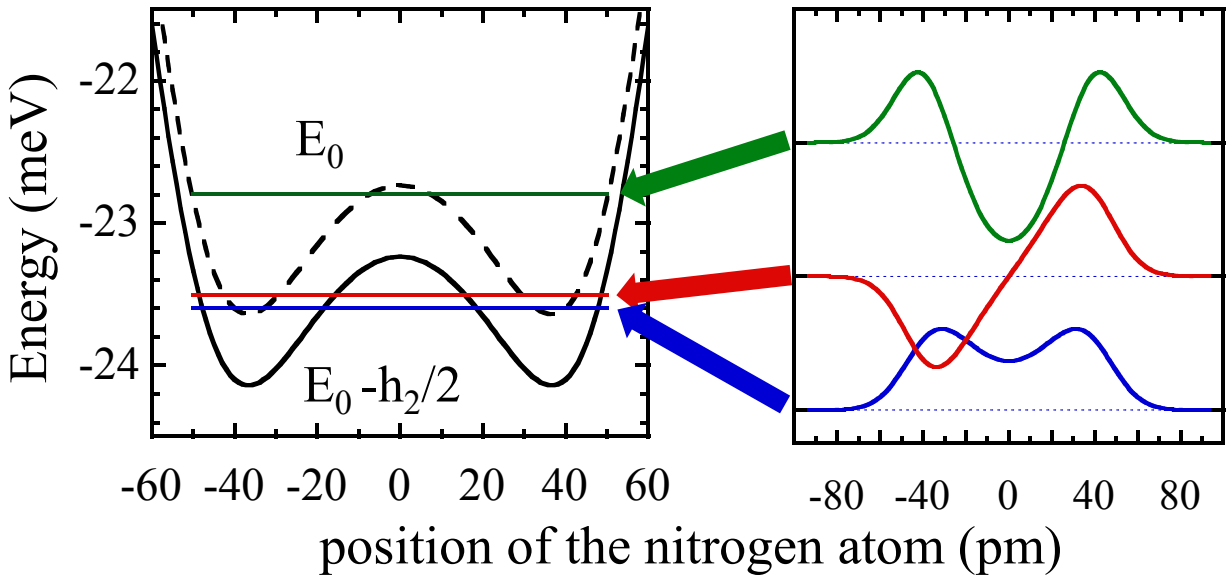

Figure 8.1: Left: Potential energy of the ammonia molecule E_0 (dashed line), the collective potential $E_0 - h_2$ (solid line), and the eigenenergies of the lowest three states (horizontal lines). Right: wave functions of the lowest three states.

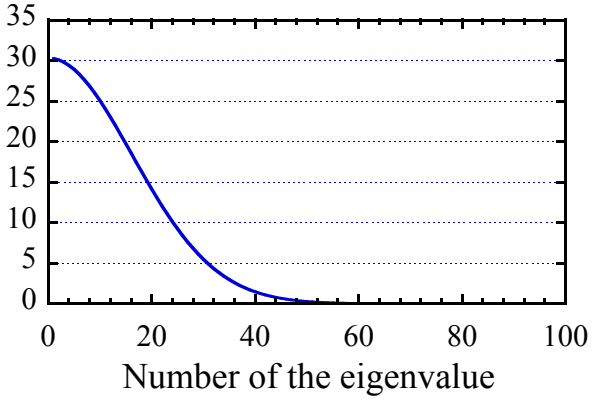

Figure 8.2:

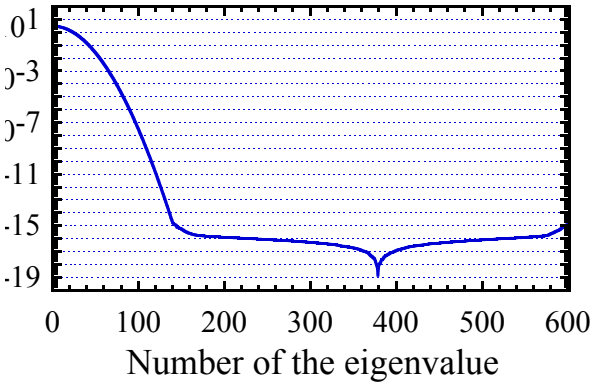

Figure 8.3:

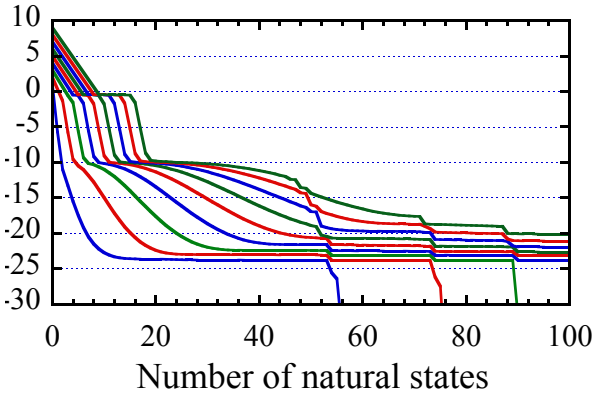

Figure 8.4:

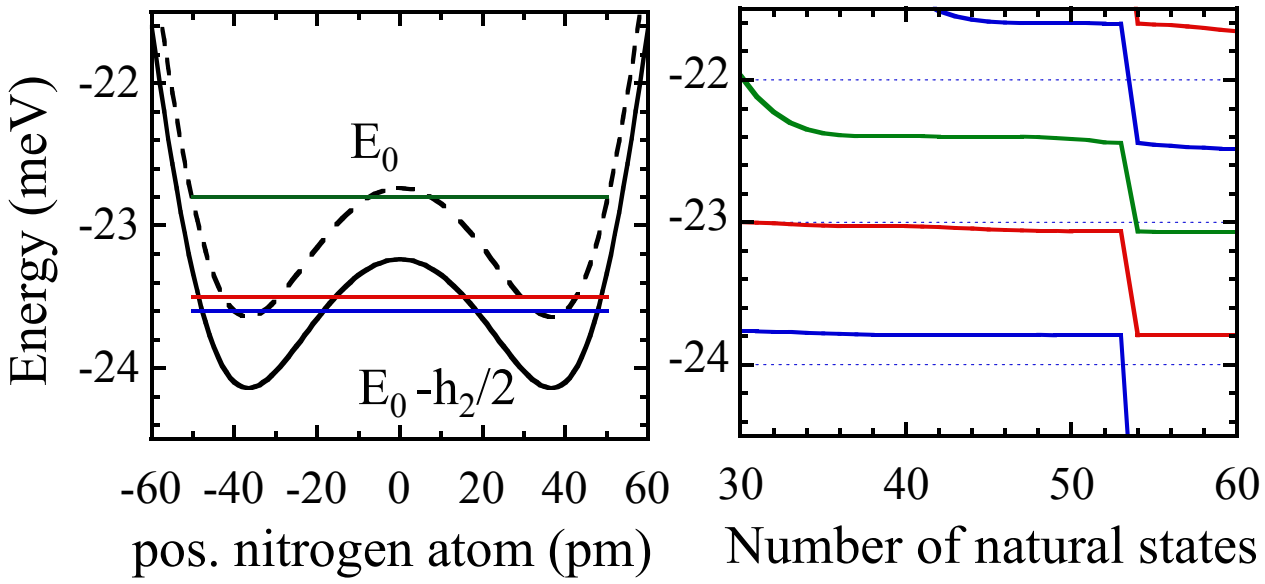

Figure 8.5: Left: Potential energy of the ammonia molecule E_0 (dashed line), the collective potential $E_0 - h_2$ (solid line), and the eigenenergies of the lowest three states (horizontal lines). Right: Hill-Wheeler eigenenergies of the lowest three states.

Lecture 9

Large Amplitude Collective Motion [Week 2 day 4]

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9.1 Adiabatic Time-Dependent Hartree-Fock Theory

9.1.1 The TDHF Equation

Define a time-dependent one-body density matrix as

$$\rho_{ji}(t) = \langle \Psi(t) | c_i^\dagger c_j | \Psi(t) \rangle, \tag{9.1}$$

where $|\Psi(t)\rangle$ is solution to the time-dependent, many-body Schrödinger equation

$$i\hbar \frac{\partial |\Psi\rangle}{\partial t} = \hat{H} |\Psi(t)\rangle. \tag{9.2}$$

Take time-derivative of density matrix and use Schrödinger equation to find

$$i\hbar\frac{\partial\rho_{ji}}{\partial t} = \langle\Psi(t)|[c_i^\dagger c_j, \hat{H}]|\Psi(t)\rangle \tag{9.3}$$

Use the Wick theorem to derive the time-dependent Hartree-Fock (TDHF) equation

$$i\hbar\dot{\rho} = [h[\rho], \rho], \tag{9.4}$$

where

- the wavefunction remains a Slater determinant at all times;
- the total energy is conserved, $E(t) = E$;
- the density is neither time-even nor time-odd: cannot be interpreted as a generalized coordinate (or a generalized momentum).

9.1.2 The ATDHF Equations

9-1: Expansion of the density matrix

The TDHF density matrix can be expanded around a reference density $\rho^{(0)}$

$$\hat{\rho}(t) = e^{i\hat{\chi}(t)}\hat{\rho}^{(0)}(t)e^{-i\hat{\chi}(t)}. \tag{9.5}$$

where $\hat{\chi} \equiv \hat{\chi}(t)$ is a *one-body, hermitian, time-even, time-dependent* operator and

- in the context of large-amplitude collective motion, the $\hat{\rho}^{(0)}(t)$ is a *time-even, time-dependent* density;
- in the derivations of the RPA equations, it is the *static* HF density;
- in the derivations of the stability matrix of the HF equation, the density is also the static HF density and $\hat{\chi}$ is time-independent.

Adiabatic approximation: the operator $\hat{\chi}$ is "small" with respect to unity.

Use transformation (9.5) and expand up to second order in χ

$$\hat{\rho}(t) = \hat{\rho}^{(0)}(t) + \hat{\rho}^{(1)}(t) + \hat{\rho}^{(2)}(t) + \dots \tag{9.6}$$

First and second order terms

$$\begin{cases} \hat{\rho}^{(1)}(t) = i\left[\hat{\chi}(t), \hat{\rho}^{(0)}(t)\right], \\ \hat{\rho}^{(2)}(t) = \frac{1}{2}\left[\left[\hat{\chi}(t), \hat{\rho}^{(0)}(t)\right], \hat{\chi}(t)\right]. \end{cases} \tag{9.7}$$

Both the density $\hat{\rho}^{(0)}(t)$ and the operator $\hat{\chi}(t)$ are hermitian and time-even

$$\begin{aligned} \hat{T}\hat{\rho}^{(0)}(t)\hat{T}^\dagger &= \hat{\rho}^{(0)}(t), \qquad & \hat{\rho}^{(0)\dagger}(t) &= \hat{\rho}^{(0)}(t), \\ \hat{T}\hat{\chi}(t)\hat{T}^\dagger &= \hat{\chi}(t), & \hat{\chi}^\dagger(t) &= \hat{\chi}(t). \end{aligned} \tag{9.8}$$

Time-dependent mean-field (general case of an energy functional not derived from a genuine two-body or more potential)

$$h_{ij}(t) = t_{ij} + \Gamma_{ij}(t), \quad \Gamma_{ij}(t) = \sum_{kl} 2\frac{\partial^2 E}{\partial\rho_{kl}\partial\rho_{ji}}\rho_{kl}(t). \tag{9.9}$$

9-2: ATDHF equations

Introducing expansion (9.6) into the TDHF equation (9.4), we classify the terms by their properties with respect to time-reversal and obtain the following to sets of equations

$$\begin{aligned} &i\hbar\dot{\hat{\rho}}^{(0)} = [\hat{h}^{(0)}, \hat{\rho}^{(1)}] + [\hat{\Gamma}^{(1)}, \hat{\rho}^{(0)}], && \text{(time-odd)} \\ &i\hbar\dot{\hat{\rho}}^{(1)} = [\hat{h}^{(0)}, \hat{\rho}^{(0)}] + [\hat{h}^{(0)}, \hat{\rho}^{(2)}] + [\hat{\Gamma}^{(1)}, \hat{\rho}^{(1)}] + [\hat{\Gamma}^{(2)}, \hat{\rho}^{(0)}], && \text{(time-even)} \end{aligned} \tag{9.10}$$

with

$$\hat{\Gamma}^{(1)}_{ij} = 2\frac{\partial^2 E}{\partial\rho_{ji}\partial\rho_{mn}}\rho^{(1)}_{mn} \ \ (\equiv \mathrm{Tr}\ \hat{v}\hat{\rho}^{(1)}), \qquad \hat{\Gamma}^{(2)}_{ij} = 2\frac{\partial^2 E}{\partial\rho_{ji}\partial\rho_{mn}}\rho^{(2)}_{mn} \tag{9.11}$$

Remarks

- ATDHF equations are self-consistent and determine simultaneously $\hat{\rho}^{(0)}(t)$ and $\hat{\chi}(t)$
- If $\hat{\chi} \to 0$, then $\hat{\rho}^{(0)}(t) \equiv \hat{\rho}^{(0)}$ and second ATDHF equation becomes $[\hat{h}^{(0)}, \hat{\rho}^{(0)}] = 0$.
- If $\hat{\chi}(t) \neq 0$, $[\hat{h}^{(0)}(t), \hat{\rho}^{(0)}(t)]$ is second order in $\hat{\chi}(t)$, see the second ATDHF equation. By assumption, it should be small at all times t: $\rho^{(0)}(t)$ is close to a HF solution.

ATDHF basis is the basis that simultaneously diagonalizes $\hat{\rho}^{(0)}(t)$, $\hat{h}^{(0)}_{hh}(t)$, and $\hat{h}^{(0)}_{pp}(t)$. The eigenvalues of $\hat{h}^{(0)}_{hh}(t)$ are called hole energies, those of $\hat{h}^{(0)}_{pp}(t)$ are called particle energies. The density $\hat{\rho}^{(0)}(t)$ being a projector, its eigenvalues are 0 or 1 as usual.

9-3: Collective momentum and velocity

By analogy with classical mechanics ($\boldsymbol{p} = m\boldsymbol{v}$), the time-dependent, time-even odd density $\dot{\rho}^{(0)}$ plays the role of a collective velocity, while χ is the associated collective momentum. They are related by a matrix which plays the role of a collective inertia (=inverse of a mass)

$$\hbar \begin{pmatrix} \dot{\rho}^{(0)}_{ph} \\ \dot{\rho}^{(0)*}_{ph} \end{pmatrix} = \begin{pmatrix} A_{ph,p'h'} & -B_{ph,p'h'} \\ -B^*_{ph,p'h'} & A^*_{ph,h'p'} \end{pmatrix} \begin{pmatrix} \chi_{p'h'} \\ \chi^*_{p'h'} \end{pmatrix} \tag{9.12}$$

with

$$\begin{aligned} A_{ph,p'h'} &= (e_p - e_h)\delta_{hh'}\delta_{pp'} + 2\frac{\partial^2 E}{\partial\rho_{hp}\partial\rho_{p'h'}} \\ B_{ph,p'h'} &= 2\frac{\partial^2 E}{\partial\rho_{hp}\partial\rho_{h'p'}} \end{aligned} \tag{9.13}$$

This matrix is the QRPA matrix.

Second order expansion of the energy with respect to χ

$$E(t) = E^{(0)}(t) + E^{(1)}(t) + E^{(2)}(t). \tag{9.14}$$

Concatenation of the ph and hp elements of operators into vectors

$$\chi = \begin{pmatrix} \chi_{ph} \\ \chi^*_{ph} \end{pmatrix}, \quad \chi^\dagger = (\chi^*_{ph}, \chi_{ph}). \tag{9.15}$$

Collective kinetic energy ($\mathcal{K} \equiv E^{(2)}$)

$$\mathcal{K} = \frac{1}{2}\mathrm{Tr}\left(\chi^\dagger \mathcal{M}\chi\right) \tag{9.16}$$

with

$$\mathcal{M} = \begin{pmatrix} +A_{ph,p'h'} & -B_{ph,p'h'} \\ -B^*_{ph,p'h'} & +A^*_{ph,p'h'} \end{pmatrix} \tag{9.17}$$

9.1.3 The Inertia Tensor

Cranking approximation: neglect the "residual" interaction

$$\mathcal{M} = \begin{pmatrix} e_p - e_h & 0 \\ 0 & e_p - e_h \end{pmatrix} \tag{9.18}$$

9-4: Inglis formula

The general expression (9.16) for the collective inertia becomes

$$\mathcal{K} = \hbar^2 \sum_{ph} \frac{|\langle p|\dot{\hat{\rho}}^{(0)}|h\rangle|^2}{e_p - e_h}, \tag{9.19}$$

which is known as the Inglis formula.

Reduction of number of freedom

$$\hat{\rho}^{(0)}(t) \equiv \hat{\rho}^{(0)}(\boldsymbol{q}(t)) = \hat{\rho}^{(0)}(q_1(t), \ldots, q_n(t)), \tag{9.20}$$

where $\boldsymbol{q} = (q_1, \ldots, q_n)$ is a set of n collective variables that carry all the time-dependence

Derivative of the density

$$\dot{\hat{\rho}}^{(0)} = \sum_{\mu} \dot{q}_\mu \frac{\partial \hat{\rho}^{(0)}}{\partial q_\mu}. \tag{9.21}$$

Classical form of the kinetic energy (at cranking approximation)

$$\mathcal{K} = \frac{1}{2} \sum_{\mu\nu} \mathsf{M}_{\mu\nu} \dot{q}_\mu \dot{q}_\nu \tag{9.22}$$

Inertia tensor

$$\mathsf{M}_{\mu\nu} = 2\hbar^2 \sum_{ph} \frac{\langle p|\frac{\partial \hat{\rho}^{(0)}}{\partial q_\mu}|h\rangle\langle h|\frac{\partial \hat{\rho}^{(0)}}{\partial q_\nu}|p\rangle}{e_p - e_h}. \tag{9.23}$$

9-5: Collective path

The ATDHF equations provide a closed set of self-consistent equations. At convergence, they determine both the entire sequence of density matrices $\{\rho^{(0)}(t)\}_{t=t_1,\ldots,t_N}$, known as the collective path, and the inertia tensor along that path. Often, one sets the collective path beforehand using HF solutions

$$[\hat{h}^{(0)} - \boldsymbol{\lambda}\hat{\boldsymbol{q}}, \hat{\rho}^{(0)}] = 0, \Rightarrow \rho^{(0)} \equiv \rho^{(0)}(\boldsymbol{q}) \tag{9.24}$$

9.1.4 Perturbative Cranking Inertia

Additional approximation (perturbative): obtain an expression for the collective inertia which is local in the coordinate space, i.e., only depends on the point $\boldsymbol{q}$.

Taylor expansion of the density at point $\boldsymbol{q} + \delta\boldsymbol{q}$

$$\hat{\rho}(\boldsymbol{q} + \delta\boldsymbol{q}) = \rho^{(0)}(\boldsymbol{q}) + \delta\boldsymbol{q} \frac{\partial \hat{\rho}}{\partial \boldsymbol{q}}, \tag{9.25}$$

leads to a perturbation of the HF Hamiltonian, $\hat{h}^{(0)} \to \hat{h} = \hat{h}^{(0)} + \delta\hat{h}$, and correspondingly of the vector of Lagrange parameters $\boldsymbol{\lambda} \to \boldsymbol{\lambda} + \delta\boldsymbol{\lambda}$.

Use RPA theory to relate the variations $\delta\boldsymbol{q}$ and $\delta\hat{\rho}$ (which defines the first-order term of the Taylor expansion) to $\delta\boldsymbol{\lambda}$ and express the derivative $\delta\hat{\rho}/\delta\boldsymbol{q}$ as a function of the RPA matrix (see exercises)

9-6: Perturbative cranking inertia tensor

The perturbative expression is built on top of the cranking approximation, i.e., it is still assumed that the RPA matrix is diagonal. We find

$$\mathsf{M} = 2\hbar^2[\mathsf{M}^{(1)}]^{-1}\mathsf{M}^{(3)}[\mathsf{M}^{(1)}]^{-1}. \tag{9.26}$$

At the cranking approximation, the inertia tensor for the system protons + neutrons is the sum of the two,

$$\mathsf{M}_{\mu\nu} = \mathsf{M}^{(n)}_{\mu\nu} + \mathsf{M}^{(p)}_{\mu\nu} \tag{9.27}$$

At the perturbative cranking approximation, the total tensor of inertia is given by the same formula (9.26),

$$\mathsf{M} = 2\hbar^2[\mathsf{M}^{(1)}]^{-1}\mathsf{M}^{(3)}[\mathsf{M}^{(1)}]^{-1}, \tag{9.28}$$

only each moment is the sum of the proton and neutron contribution.

9.2 The ATDHFB Approximation: Extension to Superfluid Systems

TDHFB equation

$$i\hbar\dot{\hat{\mathcal{R}}} = [\hat{\mathcal{H}}, \hat{\mathcal{R}}], \tag{9.29}$$

HFB matrix and generalized density

$$\mathcal{H} = \begin{pmatrix} h-\lambda & \Delta \\ -\Delta^* & -h^*+\lambda \end{pmatrix}, \qquad \mathcal{R} = \begin{pmatrix} \rho & \kappa \\ -\kappa^* & 1-\rho^* \end{pmatrix}, \tag{9.30}$$

Perturbation of the generalized density

$$\hat{\mathcal{R}}(t) = e^{i\hat{\chi}(t)}\hat{\mathcal{R}}^{(0)}(t)e^{-i\hat{\chi}(t)}, \tag{9.31}$$

Second order expansion of the generalized density

$$\hat{\mathcal{R}}(t) = \hat{\mathcal{R}}^{(0)}(t) + \hat{\mathcal{R}}^{(1)}(t) + \hat{\mathcal{R}}^{(2)}(t) + \mathcal{O}(\hat{\chi}^3), \tag{9.32}$$

with the analog of Eqs.(9.8),

$$\begin{aligned}\hat{\mathcal{R}}^{(1)}(t) &= i\left[\hat{\chi}(t), \hat{\mathcal{R}}^{(0)}(t)\right], \\ \hat{\mathcal{R}}^{(2)}(t) &= \frac{1}{2}\left[\left[\hat{\chi}(t), \hat{\mathcal{R}}^{(0)}(t)\right], \hat{\chi}(t)\right].\end{aligned} \tag{9.33}$$

Second order expansion of the HFB matrix

$$\hat{\mathcal{H}}(t) = \hat{\mathcal{H}}^{(0)}(t) + \hat{\mathcal{H}}^{(1)}(t) + \hat{\mathcal{H}}^{(2)}(t) + \mathcal{O}(\hat{\chi}^3), \tag{9.34}$$

ATDHFB equations

$$\begin{aligned} i\hbar\dot{\hat{\mathcal{R}}}^{(0)} &= [\hat{\mathcal{H}}^{(0)}, \hat{\mathcal{R}}^{(1)}] + [\hat{\mathcal{H}}^{(1)}, \hat{\mathcal{R}}^{(0)}], && \text{(time-odd)} \\ i\hbar\dot{\hat{\mathcal{R}}}^{(1)} &= [\hat{\mathcal{H}}^{(0)}, \hat{\mathcal{R}}^{(0)}] + [\hat{\mathcal{H}}^{(0)}, \hat{\mathcal{R}}^{(2)}] + [\hat{\mathcal{H}}^{(1)}, \hat{\mathcal{R}}^{(1)}] + [\hat{\mathcal{H}}^{(2)}, \hat{\mathcal{R}}^{(0)}]. && \text{(time-even)}\end{aligned} \tag{9.35}$$

Notations

$$\mathcal{H}^{(0)} = \begin{pmatrix} h^{(0)} - \lambda & \Delta^{(0)} \\ -\Delta^{(0)*} & -h^{(0)*} + \lambda \end{pmatrix}, \; \mathcal{H}^{(1)} = \begin{pmatrix} \Gamma^{(1)} & \Delta^{(1)} \\ -\Delta^{(1)*} & -\Gamma^{(1)*} \end{pmatrix}, \; \mathcal{H}^{(2)} = \begin{pmatrix} \Gamma^{(2)} & \Delta^{(2)} \\ -\Delta^{(2)*} & -\Gamma^{(2)*} \end{pmatrix} \tag{9.36}$$

with

$$\begin{aligned} \Gamma^{(1)}_{ij} &= \sum_{kl} \bar{v}_{ikjl}\rho^{(1)}_{lk}, \quad \Delta^{(1)}_{ij} = \frac{1}{2}\sum_{kl} \bar{v}_{ijkl}\kappa^{(1)*}_{kl}, \\ \Gamma^{(2)}_{ij} &= \sum_{kl} \bar{v}_{ikjl}\rho^{(2)}_{lk}, \quad \Delta^{(2)}_{ij} = \frac{1}{2}\sum_{kl} \bar{v}_{ijkl}\kappa^{(2)*}_{kl}. \end{aligned} \tag{9.37}$$

ATDHFB basis: basis that diagonalizes the generalized density $\hat{\mathcal{R}}^{(0)}$

Structure of $\tilde{\mathcal{H}}^{(0)}$

$$\tilde{\mathcal{H}}^{(0)} = \begin{pmatrix} E & H^{(0)}_{12} \\ H^{(0)}_{21} & -E \end{pmatrix}. \tag{9.38}$$

Notation

$$\tilde{\chi} = \begin{pmatrix} \chi_{11} & \chi_{12} \\ \chi_{21} & \chi_{22} \end{pmatrix}, \tag{9.39}$$

First ATDHFB equation in the ATDHFB basis

$$\hbar \begin{pmatrix} \dot{R}^{12}_{ij} \\ \dot{R}^{12*}_{ij} \end{pmatrix} = \begin{pmatrix} A & B \\ B^* & A^* \end{pmatrix} \begin{pmatrix} \chi^{12}_{ij} \\ \chi^{12*}_{ij} \end{pmatrix} \tag{9.40}$$

Next step: express the energy $E[\mathcal{R}]$ up to second order

$$E[\mathcal{R}] = E_{\text{HFB}} + \frac{1}{4}(\chi^{12*}\chi^{12}) \begin{pmatrix} A & B \\ B^* & A^* \end{pmatrix} \begin{pmatrix} \chi^{12} \\ \chi^{12*} \end{pmatrix} \tag{9.41}$$

Collective kinetic energy

$$\mathcal{K} = \frac{1}{4}\mathrm{Tr}\left(\chi^\dagger \mathcal{M}\chi\right) = \frac{\hbar^2}{4}\mathrm{Tr}\left(\dot{\mathcal{R}}^\dagger \mathcal{M}^{-1}\dot{\mathcal{R}}\right) \tag{9.42}$$

As before, introduce collective variables and assume that

$$\dot{\mathcal{R}} \equiv \sum_b \dot{q}_b \frac{\partial \mathcal{R}}{\partial q_b} \tag{9.43}$$

Then, use again QRPA theory to express $\partial\mathcal{R}/\partial q_b$ as function of matrix elements of the operators associated with q_b,

$$\mathcal{M}\begin{pmatrix} \mathcal{R}^{12} \\ \mathcal{R}^{12*} \end{pmatrix} = \sum_b \left[M^{(1)}\right]^{-1}_{ab} \mathcal{M}^{-1}\begin{pmatrix} Q_b^{12} \\ Q_b^{12*} \end{pmatrix} \tag{9.44}$$

Collective inertia tensor at the ATDHFB approximation in full glory

$$\mathsf{M}_{\mu\nu} = \sum_{ab}\left[M^{(1)}\right]^{-1}_{\mu a}(Q_a^{12*}Q_b^{12})\mathcal{M}^{-3}\begin{pmatrix} Q_b^{12} \\ Q_b^{12*} \end{pmatrix}\left[M^{(1)}\right]^{-1}_{b\nu} \tag{9.45}$$

9-7: ATDHFB Inertia

The full, exact calculation of the collective inertia at the ATDHFB approximation requires inverting the full QRPA matrix for a deformed nucleus.

9.3 Gaussian overlap approximation of the generator coordinate method

Recall the general GCM ansatz for the wave function

$$|\Psi\rangle = \int d\boldsymbol{a} f(\boldsymbol{a})|\phi_{\boldsymbol{a}}\rangle, \tag{9.46}$$

where $\boldsymbol{a} = (a_1, \ldots, a_N)$ is a vector of collective variables, and $|\phi_{\boldsymbol{a}}\rangle$ a set of many-body wave functions that are known (for example, HFB solutions under the constraints given by $\boldsymbol{a}$).

Recall the norm and Hamiltonian overlaps

$$\mathcal{H}(\mathbf{a},\mathbf{a}') = \langle\phi_{\mathbf{a}}|\hat{H}|\phi_{\mathbf{a}'}\rangle, \quad \mathcal{I}(\mathbf{a},\mathbf{a}') = \langle\phi_{\mathbf{a}}|\phi_{\mathbf{a}'}\rangle \tag{9.47}$$

9.3.1 The GOA approximation

9-8: Gaussian overlap approximation (GOA)

In the Gaussian overlap approximation, we assume that the norm overlap reads

$$\mathcal{I}(\mathbf{a},\mathbf{a}') = \exp\left[-\frac{1}{2}(\mathbf{a}-\mathbf{a}')\mathsf{G}(\bar{\mathbf{a}})(\mathbf{a}-\mathbf{a}')\right]. \tag{9.48}$$

with $\bar{\mathbf{a}} = (\mathbf{a}+\mathbf{a}')/2$ and $\gamma(\mathbf{a}) = \det(\mathsf{G}(\mathbf{a}))$

Reduced Hamiltonian

$$\mathcal{H}(\mathbf{a},\mathbf{a}') = \mathcal{I}(\mathbf{a},\mathbf{a}')h(\mathbf{a},\mathbf{a}'), \tag{9.49}$$

Derivatives at point $\mathbf{a} = \mathbf{a}' = \mathbf{q}$

$$h_{\mathbf{aa}} \equiv h_{a_k a_l} = \left.\frac{\partial^2 h(\mathbf{a},\mathbf{a}')}{\partial a_k \partial a_l}\right|_{\mathbf{a}=\mathbf{a}'=\mathbf{q}}, \quad h_{\mathbf{aa}} \equiv h_{a_k a'_l} = \left.\frac{\partial^2 h(\mathbf{a},\mathbf{a}')}{\partial a_k \partial a'_l}\right|_{\mathbf{a}=\mathbf{a}'=\mathbf{q}} \tag{9.50}$$

Procedure: expand the reduced Hamiltonian up to second order in $\mathbf{a}$ and $\mathbf{a}'$ around point $\mathbf{a} = \mathbf{a}' = \mathbf{q}$ by using the fact that

$$\langle\Psi|\hat{H}|\Psi\rangle = \int d\mathbf{a}\int d\mathbf{a}'\int d\mathbf{q} f^*(\mathbf{a})\mathcal{I}^{1/2}(\mathbf{a},\mathbf{q})h(\mathbf{a},\mathbf{a}')f(\mathbf{a}')\mathcal{I}^{1/2}(\mathbf{q},\mathbf{a}'), \tag{9.51}$$

introduce

$$g(\mathbf{q}) = \int d\mathbf{a}\mathcal{I}^{1/2}(\mathbf{q},\mathbf{a})f(\mathbf{a}) \tag{9.52}$$

and express terms such as $(\mathbf{a}-\mathbf{a}')$ as functions of the derivatives of $\mathcal{I}^{1/2}$ with respect to $\mathbf{q}$

9-9: Collective Hamiltonian and Inertia

In the GOA approximation, we can extract a collective Schrödinger equation that involves the collective Hamiltonian

$$\mathcal{H}_{\text{coll}}(\mathbf{q}) = -\frac{1}{2}\frac{\partial}{\partial\mathbf{q}}\mathsf{B}\frac{\partial}{\partial\mathbf{q}} + V_{\text{coll}}(\mathbf{q}) \tag{9.53}$$

with the collective potential and collective inertia tensor given by

$$\begin{aligned} V_{\text{coll}}(\mathbf{q}) &= V(\mathbf{q}) - \frac{1}{2}\mathsf{G}^{-1}h_{\mathbf{aa}'} + \frac{1}{8}\mathsf{G}^{-1}\frac{\partial^2 h_{\mathbf{aa}}}{\partial\mathbf{q}^2} \\ \mathsf{B} &= \frac{1}{2}\mathsf{G}^{-1}(h_{\mathbf{aa}'} - h_{\mathbf{aa}})\mathsf{G}^{-1} \end{aligned} \tag{9.54}$$

Local collective Hamiltonian for coordinate-dependent metric

$$\hat{\mathcal{H}}_{\text{coll}}(\mathbf{a}) = -\frac{\hbar^2}{2\sqrt{\gamma(\mathbf{a})}}\sum_{kl}\frac{\partial}{\partial a_k}\sqrt{\gamma(\mathbf{a})}\mathsf{B}_{kl}(\mathbf{a})\frac{\partial}{\partial a_l} + V(\mathbf{a}). \tag{9.55}$$

Collective inertia tensor B for coordinate-dependent metric

$$\mathsf{B}_{ij}(\mathbf{q}) = \frac{1}{2\hbar^2}\sum_{kl}\mathsf{G}^{-1}_{ik}(\mathbf{q})\left[h_{\mathbf{aa}'} - h_{\mathbf{aa}} + \Gamma^n_{kl}(\mathbf{a})\frac{\partial h(\mathbf{a},\mathbf{a}')}{\partial a_n}\bigg|_{\mathbf{a}=\mathbf{a}'=\mathbf{q}}\right]\mathsf{G}^{-1}_{lj}(\mathbf{q}). \tag{9.56}$$

Reminder: Christoffel symbol

$$\Gamma^n_{kl}(\mathbf{a}) = \frac{1}{2}\sum_i \mathsf{G}^{-1}_{ni}(\mathbf{a})\left(\frac{\partial \mathsf{G}_{ki}}{\partial a_l} + \frac{\partial \mathsf{G}_{il}}{\partial a_k} - \frac{\partial \mathsf{G}_{lk}}{\partial a_i}\right). \tag{9.57}$$

All derivatives in the previous equation are evaluated at $\mathbf{a} = \mathbf{a}' = \mathbf{q}$.

9.3.2 Local approximation

Using the Thouless theorem, the action of collective momentum on HFB state is

$$\hat{P}_k|\Phi_\mathbf{a}\rangle = \sum_{\mu<\nu}\left[P^{12}_{k;\mu\nu}\beta^\dagger_\mu\beta^\dagger_\nu + P^{21}_{k;\mu\nu}\beta_\mu\beta_\nu\right]|\Phi_\mathbf{a}\rangle \tag{9.58}$$

with $P^{21}_{k;\mu\nu} = P^{12*}_{k;\nu\mu}$

Reminder: HFB equations at point $\mathbf{a}$

$$[\mathcal{H}(\mathbf{a}) - \sum_a \lambda_a\mathcal{Q}_a, \mathcal{R}(\mathbf{a})] = 0, \tag{9.59}$$

where $\mathcal{Q}_a$ is the matrix of the constraint operator $\hat{Q}_a$ in the double sp basis and λ_a is the Lagrange parameter for the collective variable a ($a \equiv a_k$ for $k = 1,\ldots,N$).

Small variations

$$\begin{aligned}\mathcal{H}(\mathbf{a}+\delta\mathbf{a}) &= \mathcal{H}(\mathbf{a}) + \mathcal{H}_1,\\ \mathcal{R}(\mathbf{a}+\delta\mathbf{a}) &= \mathcal{R}(\mathbf{a}) + \mathcal{R}_1,\\ \lambda_a(\mathbf{a}+\delta\mathbf{a}) &= \lambda_a(\mathbf{a}) + \delta\lambda_a.\end{aligned} \tag{9.60}$$

HFB equation to first order in $\delta\mathbf{a}$

$$[\mathcal{R}_1, \mathcal{H}(\mathbf{a}) - \sum_a \lambda_a\mathcal{Q}_a] + [\mathcal{R}(\mathbf{a}), \mathcal{H}_1] = \sum_a \delta\lambda_a[\mathcal{R}(\mathbf{a}), \mathcal{Q}_a]. \tag{9.61}$$

QRPA

$$\mathcal{M}\begin{pmatrix} R^{12} \\ R^{12\,*}\end{pmatrix} = \sum_a \delta\lambda_a\begin{pmatrix} Q^{12}_a \\ Q^{12\,*}_a\end{pmatrix}, \tag{9.62}$$

Collective momentum as function of collective variable at point $\mathbf{q}$

$$\begin{pmatrix} P^{12}_a \\ -P^{12*}_a\end{pmatrix} = \sum_b [\mathsf{M}^{(1)}]^{-1}_{ab}\tilde{\mathcal{M}}^{-1}\begin{pmatrix} Q^{12}_b \\ Q^{12\,*}_b\end{pmatrix}. \tag{9.63}$$

where $\tilde{\mathcal{M}}$ is just so slightly different from the QRPA matrix $\mathcal{M}$

$$\tilde{\mathcal{M}} = \begin{pmatrix} A & -B \\ -B^* & A^* \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \mathcal{M} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{9.64}$$

Definition of the overlap kernel G_{ab}

$$\mathsf{G}_{ab}(\mathbf{q}) = \frac{1}{\hbar^2}\langle\Phi_{\mathbf{q}}|\hat{P}_k\hat{P}_l|\Phi_{\mathbf{q}}\rangle, \tag{9.65}$$

In the cranking approximation of the GCM, the inertia tensor is expressed entirely as function of the moments

$$\mathsf{B} = \mathsf{M}^{(1)}[\mathsf{M}^{(2)}]^{-1}\tilde{\mathsf{M}}^{(1)}[\mathsf{M}^{(2)}]^{-1}\mathsf{M}^{(1)}. \tag{9.66}$$

Same moments as in ATDHFB

$$\mathsf{M}^{(K)}_{ab} = \mathfrak{Re}\sum_{\mu\nu}\frac{\langle\mu\nu|\hat{Q}_a|0\rangle\langle 0|\hat{Q}_b|\mu\nu\rangle}{(E_\mu + E_\nu)^K}. \tag{9.67}$$

9-10: Collective inertia at the perturbative cranking

In the perturbative (=local) cranking approximation of the GCM, the inertia tensor is expressed entirely as function of the moments

$$\mathsf{B} = \mathsf{M}^{(1)}[\mathsf{M}^{(2)}]^{-1}\mathsf{M}^{(1)}[\mathsf{M}^{(2)}]^{-1}\mathsf{M}^{(1)}. \tag{9.68}$$

with the metric tensor given by

$$\mathsf{G} = \frac{1}{2}[\mathsf{M}^{(1)}]^{-1}\mathsf{M}^{(2)}[\mathsf{M}^{(1)}]^{-1}. \tag{9.69}$$

Alternative expression

$$\mathsf{B} = \frac{1}{4}\mathsf{G}^{-1}[\mathsf{M}^{(1)}]^{-1}\mathsf{G}^{-1}. \tag{9.70}$$

9.4 Exercises

9.4.1 ATDHF

Exercise 21.

Show that in the basis that diagonalizes $\hat{\rho}^{(0)}(t)$ at time t, any operator $\hat{A}$ can be written

$$\hat{A} = \hat{A}_{hp} + \hat{A}_{ph} \tag{9.71}$$

where $\hat{A}_{hp} = \hat{\rho}^{(0)}(t)\hat{A}\hat{\sigma}^{(0)}(t)$ (and similarly with $\hat{A}_{ph}$), with

$$\begin{aligned} \hat{\rho}^{(0)}(t) &= \sum_h |h\rangle\langle h|, \\ \hat{\sigma}^{(0)}(t) &= \sum_p |p\rangle\langle p| = 1 - \hat{\rho}^{(0)}(t). \end{aligned} \tag{9.72}$$

and $|h\rangle$ an eigenvector of $\hat{\rho}^{(0)}(t)$ with eigenvalue 1 and $|p\rangle$ an eigenvector with eigenvalue 0.

Exercise 22.

Show hat we can find at all times t a basis that simultaneously diagonalizes $\hat{\rho}^{(0)}(t)$, $\hat{h}^{(0)}_{hh}(t)$, and $\hat{h}^{(0)}_{pp}(t)$.

Exercise 23.

Show that, in the ATDHF basis, the matrix of $\rho^{(1)}$ reads

$$\rho^{(1)} = \begin{pmatrix} 0 & +i\chi_{ph} \\ -i\chi_{hp} & 0 \end{pmatrix}. \tag{9.73}$$

Exercise 24.

Show that the first ATDHF equation can be written

$$\begin{aligned} \hbar\dot{\rho}^{(0)}_{ph} &= (e_p - e_h)\chi_{ph} - i\Gamma^{(1)}_{ph} \\ \hbar\dot{\rho}^{(0)}_{hp} &= (e_p - e_h)\chi_{hp} + i\Gamma^{(1)}_{hp} \end{aligned} \tag{9.74}$$

Exercise 25.

Show that the first term of $E^{(2)}$ reads

$$\text{tr}\ \hat{h}^{(0)}\hat{\rho}^{(2)} = \frac{1}{2}\sum_{ph}(e_p - e_h)\chi_{ph}\chi^*_{ph} + \frac{1}{2}\sum_{ph}(e_p - e_h)\chi_{ph}\chi^*_{ph}. \tag{9.75}$$

and that the second one reads

$$\text{tr}\ \hat{\rho}^{(1)}\Gamma^{(1)} = \bar{v}_{ph'hp'}\chi_{p'h'}\chi_{hp} - \bar{v}_{pp'hh'}\chi_{h'p'}\chi_{hp} - \bar{v}_{hh'pp'}\chi_{p'h'}\chi_{ph} + \bar{v}_{hp'ph'}\chi_{h'p'}\chi_{ph} \tag{9.76}$$

9.4.2 ATDHFB

Exercise 26.

Show that the perturbed static HF equation can be written

$$[\hat{h}^{(0)} - \boldsymbol{\lambda}\hat{\boldsymbol{q}}, \delta\hat{\rho}] = \delta\boldsymbol{\lambda}[\hat{\boldsymbol{q}}, \hat{\rho}^{(0)}]. \tag{9.77}$$

at first order in $\delta\hat{\rho}$ and neglecting variations of the mean field δh

---

Exercise 27.

Evaluate these commutators in the HF basis of $\hat{\rho}^{(0)}$. Recall that in that basis,

$$(\hat{h}^{(0)} - \boldsymbol{\lambda}\hat{\boldsymbol{q}})_{ij} = e_i\delta_{ij}, \quad \rho^{(0)}_{ij} = n_i\delta_{ij}, \quad Q_{\mu,ij} = \langle i|\hat{Q}_\mu|j\rangle. \tag{9.78}$$

Exercise 28.

Use the definition of the expectation value of $\hat{Q}$ to obtain a elation between δq_μ and $\delta\lambda_\nu$ that involves the moments

$$M^{(K)}_{\mu\nu} = \sum_{ph} \frac{\langle p|\hat{Q}_\mu|h\rangle\langle h|\hat{Q}_\nu|p\rangle}{(e_p - e_h)^K} \tag{9.79}$$

Exercise 29.

Show that the matrices $\tilde{\mathcal{R}}^{(1)}$ and $\tilde{\tilde{\mathcal{R}}}^{(0)}$ have the following form

$$\tilde{\mathcal{R}}^{(1)} = \begin{pmatrix} 0 & i\chi_{12} \\ -i\chi_{21} & 0 \end{pmatrix}. \tag{9.80}$$

and

$$\tilde{\tilde{\mathcal{R}}}^{(0)} = \begin{pmatrix} 0 & \dot{R}^{(0)}_{12} \\ \dot{R}^{(0)}_{21} & 0 \end{pmatrix} \tag{9.81}$$

Exercise 30.

Show that, in the s.p. basis, we have

$$\begin{aligned} \rho^{(1)} &= -iV^*\chi_{21}U^\dagger + iU\chi_{12}V^T \\ \kappa^{(1)} &= -iV^*\chi_{21}V^\dagger + iU\chi_{12}U^T \end{aligned} \tag{9.82}$$

Exercise 31.

Show that, in the s.p. basis, we have

$$\begin{aligned} H_{12}^{(1)} &= U^\dagger \Gamma^{(1)} V^* - V^\dagger \Delta^{(1)*} V^* + U^\dagger \Delta^{(1)} U^* - V^\dagger \Gamma^{(1)*} U^* \\ H_{21}^{(1)} &= V^T \Gamma^{(1)} U - U^T \Delta^{(1)*} U + V^T \Delta^{(1)} V - U^T \Gamma^{(1)*} V \end{aligned} \tag{9.83}$$

Exercise 32.

By using the special form of all these matrices in the qp basis, show that the ATDHF equation can be expressed as

$$\begin{aligned} \hbar \dot{R}_{ij}^{12} &= (E_i + E_j)\chi_{ij}^{12} - iH_{ij}^{12} \\ \hbar \dot{R}_{ji}^{12*} &= (E_i + E_j)\chi_{ji}^{12*} + iH_{ji}^{12*} \end{aligned} \tag{9.84}$$

9.4.3 GCM+GOA

Exercise 33.

Starting with the expression of the square of the norm overlap $\mathcal{I}^{1/2}(\boldsymbol{a}, \boldsymbol{a'})$ and using the property $\mathsf{G}_{ik}\mathsf{G}_{kj}^{-1} = \delta_{ij}$ (Einstein summation conventions used), show that

$$\mathsf{G}_{il}^{-1} \frac{\partial \mathcal{I}^{1/2}}{\partial a_l} = -2(\mathbf{a} - \mathbf{a}')_i \mathcal{I}^{1/2}, \tag{9.85}$$

$$\mathsf{G}_{il}^{-1} \frac{\partial \mathcal{I}^{1/2}}{\partial a'_l} = +2(\mathbf{a} - \mathbf{a}')_i \mathcal{I}^{1/2}, \tag{9.86}$$

and

$$\mathsf{G}_{ik}^{-1} \frac{\partial^2 \mathcal{I}^{1/2}}{\partial a_k \partial a_l} \mathsf{G}_{lj}^{-1} = -2\mathsf{G}_{ij}^{-1} \mathcal{I}^{1/2} + 4(\mathbf{a} - \mathbf{a}')_i (\mathbf{a} - \mathbf{a}')_j \mathcal{I}^{1/2}, \tag{9.87}$$

$$\mathsf{G}_{ik}^{-1} \frac{\partial^2 \mathcal{I}^{1/2}}{\partial a_k \partial a'_l} \mathsf{G}_{lj}^{-1} = +2\mathsf{G}_{ij}^{-1} \mathcal{I}^{1/2} + 4(\mathbf{a} - \mathbf{a}')_i (\mathbf{a} - \mathbf{a}')_j \mathcal{I}^{1/2}. \tag{9.88}$$

Exercise 34.

By using a Taylor expansion of the reduced Hamiltonian $h(\boldsymbol{a}, \boldsymbol{a'})$ at point $\mathbf{a} = \mathbf{a}' = \mathbf{q}$, express the expectation value $\langle \Psi | \hat{H} | \Psi \rangle$ of the Hamiltonian on the GCM state up to second order in $\boldsymbol{a} - \boldsymbol{q}$ and $\boldsymbol{q} - \boldsymbol{a'}$.

Exercise 35.

By using the property

$$|\Phi_{\mathbf{a}}\rangle = e^{i(\mathbf{a}-\mathbf{q})\hat{\mathbf{P}}_{\mathbf{q}}/\hbar} |\Phi_{\mathbf{q}}\rangle.$$

show that

- Time-reversal properties impose that

$$\frac{\partial}{\partial a_k}\mathcal{I}(\mathbf{a},\mathbf{a}')|_{\mathbf{a}=\mathbf{a}'=\mathbf{q}}=0. \tag{9.89}$$

- The metric tensor can be expressed as

$$\frac{1}{\hbar^2}\langle\Phi_{\mathbf{q}}|\hat{P}_k\hat{P}_l|\Phi_{\mathbf{q}}\rangle=\mathsf{G}_{kl}. \tag{9.90}$$

- The second derivatives of the Hamiltonian overlap kernels are

$$\begin{aligned}\frac{\partial^2 h(\mathbf{a},\mathbf{a}')}{\partial a_k\partial a_l}&=\left.\frac{\partial^2\mathcal{H}(\mathbf{a},\mathbf{a}')}{\partial a_k\partial a_l}\right|_{\mathbf{a}=\mathbf{a}'=\mathbf{q}}-E(\mathbf{q})\frac{\partial^2\mathcal{I}(\mathbf{a},\mathbf{a}')}{\partial a_k\partial a_l}|_{\mathbf{a}=\mathbf{a}'=\mathbf{q}},\\ \frac{\partial^2 h(\mathbf{a},\mathbf{a}')}{\partial a_k\partial a'_l}&=\left.\frac{\partial^2\mathcal{H}(\mathbf{a},\mathbf{a}')}{\partial a_k\partial a'_l}\right|_{\mathbf{a}=\mathbf{a}'=\mathbf{q}}-E(\mathbf{q})\frac{\partial^2\mathcal{I}(\mathbf{a},\mathbf{a}')}{\partial a_k\partial a'_l}|_{\mathbf{a}=\mathbf{a}'=\mathbf{q}}.\end{aligned} \tag{9.91}$$

Exercise 36.

Show that the inverse of the QRPA matrix as a similar block structure, namely,

$$\mathcal{M}^{-1}=\begin{pmatrix}C & D\\ D^* & C^*\end{pmatrix},\quad C=C^\dagger, D=D^T. \tag{9.92}$$

Exercise 37.

Using the symmetry properties of G, and the results (9.90) and (9.58), show that we can write

$$\mathsf{G}_{ab}=\frac{1}{4}\left(P^{12*}_{a;\mu\nu},-P^{12}_{a;\mu\nu}\right)\begin{pmatrix}P^{12}_{b;\mu\nu}\\ -P^{12*}_{b;\mu\nu}\end{pmatrix}, \tag{9.93}$$

where indices μ, ν run over the entire basis set.

Exercise 38.

Show that

$$h_{\mathbf{aa}'}=\sum_{i<j,\mu<\nu}P^{12*}_{k,ij}P^{12}_{l,\mu\nu}A_{ij\mu\nu}. \tag{9.94}$$

and

$$h_{\mathbf{aa}}=-\sum_{i<j,\mu<\nu}P^{12*}_{k,ij}P^{21}_{l,\mu\nu}B_{ij\nu\mu}, \tag{9.95}$$

Exercise 39.

Using the properties that $A_{ij\mu\nu}=A^*_{\mu\nu ij}$ (same for B), $B_{ij\mu\nu}=-B_{ij\nu\mu}$, and $P^{12}_{k,ij}=-P^{21*}_{k,ij}$, and after removing the restrictions on the summation indices, show that

$$h_{\mathbf{aa}'}-h_{\mathbf{aa}}=\frac{1}{4}(P^{12*}_k,P^{12}_k)\begin{pmatrix}A & B\\ B^* & A^*\end{pmatrix}\begin{pmatrix}P^{12}_l\\ P^{12*}_l\end{pmatrix}. \tag{9.96}$$

Exercise 40.

Introduce the matrix

$$\tilde{\mathcal{M}} = \begin{pmatrix} A & -B \\ -B^* & A^* \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \mathcal{M} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{9.97}$$

Show that we have

$$h_{\mathbf{aa'}} - h_{\mathbf{aa}} = \frac{1}{2}[\mathsf{M}^{(1)}]^{-1}\tilde{\mathsf{M}}^{(1)}[\mathsf{M}^{(1)}]^{-1}. \tag{9.98}$$

Lecture 10

Phenomenological nuclear functionals I [Week 2, day 5]

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10.1 The Nuclear Hamiltonian

The QCD Lagrangian is the current description of the Strong force

$$\mathcal{L} = -\frac{1}{4} F^{\alpha}_{\mu\nu} F^{\mu\nu}_{\alpha} - \sum_{n} \bar{\Psi}_n \gamma^{\mu} \left[\partial_{\mu} - i g A^{\alpha}_{\mu} t_{\alpha} \right] \Psi_n - m_n \bar{\Psi}_n \Psi_n \tag{10.1}$$

with α the index for the 8 colors, n the 6 quark flavour (u,d,s,t,b,c) index, ν, μ the quadri-coordinates. A represents the gluon vector field, Ψ the quarks wavefunctions. F is the field tensor, that is made of appropriately coupled vector fields,

$$F^{\alpha}_{\mu\nu} = \partial_{\mu} A^{\alpha}_{\nu} - \partial_{\nu} A^{\alpha}_{\mu} + C^{\alpha}_{\beta\gamma} A^{\beta}_{\mu} A^{\gamma}_{\nu} \tag{10.2}$$

the last term is the self-interaction between gluons, that is the main difference with QED and is the whole reason QCD is non perturbative (at low energies) making nuclear physics so

complicated (cf. Fig. 10.1, Cool animations at
`http://www.physics.adelaide.edu.au/theory/staff/leinweber/VisualQCD/Nobel/`) The

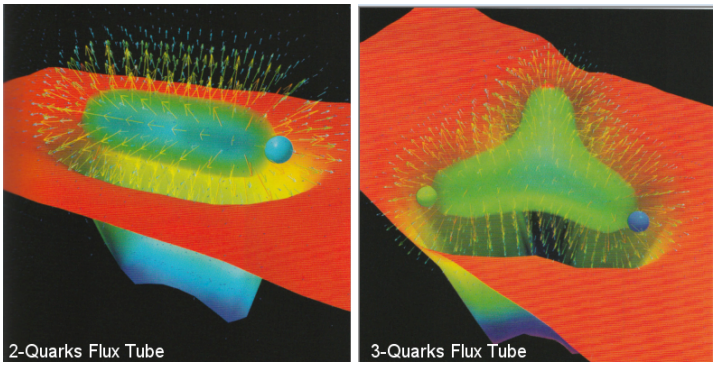

Figure 10.1: Courtesy of Derek B. Leinweber, for GlueX collaboration [18].

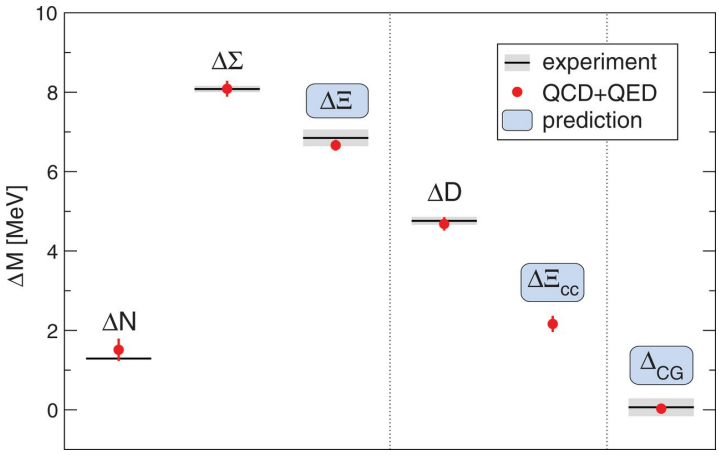

Figure 10.2: Reproduction of Hadrons masses from ab–initio [19].

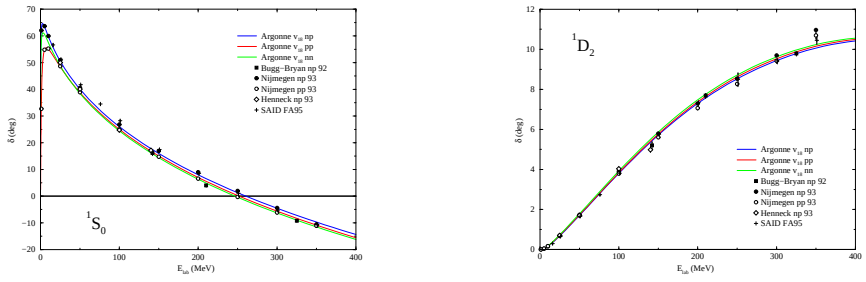

Figure 10.3: Two examples of the Phase Shifts of Argonne v_{18} compared with experimental result.

are several ways to build a low energy representation of the nuclear strong force: both phenomenological (e.g. Argonne v_{18} + Urbana IX, cf.

https://www.phy.anl.gov/theory/research/av18/) and exploiting the symmetries of the QCD–Lagrangian (the Chiral Effective Field Theory, χEFT, being one of the most promising). The nature of this bare force is inherently many–body. Moreover they are often very difficult to treat due to the presence of an hard–core (the two–body part of the interaction goes to infinity at $r \lesssim 0.4$ fm), and the interaction has to be regularized with renormalization techniques (SRG) before being used introducing non–physical cutoffs. After the regularization, and even in case of naturally soft–core potentials (e.g. NNLO$_{sat}$), this is a representation of the bare force between two (or more) nucleons in the vacuum, thus is not suited to describe the *effective* interactions between nucleons in the nucleus and then be used for Density Functionals calculations as it is.

Then we are back at the starting point of an 'unknown', effective A–body hamiltonian for the nuclear system,

$$\hat{H} = \hat{T} + \hat{V}_2(\mathbf{x}_1, \mathbf{x}_2) + \hat{V}_3(\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3) + \cdots + \hat{V}_A(\mathbf{x}_1, \cdots, \mathbf{x}_A) \tag{10.3}$$

with $\mathbf{x}$ representing $\mathbf{r}, \sigma, \tau$.

10.2 Effective pseudopotentials

10.2.1 General Two–Bodies

Let's consider the radial dependence of a general two–body interaction,

$$\langle \mathbf{r}_1' \mathbf{r}_2' | V | \mathbf{r}_1 \mathbf{r}_2 \rangle = V(\mathbf{r}_1', \mathbf{r}_2', \mathbf{r}_1, \mathbf{r}_2) \tag{10.4}$$

we can write $|\mathbf{r}_1' \mathbf{r}_2'\rangle$ as expansion,

$$|\mathbf{r}_1' \mathbf{r}_2'\rangle = |\mathbf{r}_1 \mathbf{r}_2\rangle + (\mathbf{r}_1 - \mathbf{r}_1') \frac{\partial}{\partial \mathbf{r}_1} |\mathbf{r}_1 \mathbf{r}_2\rangle + (\mathbf{r}_2 - \mathbf{r}_2') \frac{\partial}{\partial \mathbf{r}_2} |\mathbf{r}_1 \mathbf{r}_2\rangle + \cdots = e^{\frac{i}{\hbar}((\mathbf{r}_1 - \mathbf{r}_1') \cdot \mathbf{p}_1 + (\mathbf{r}_2 - \mathbf{r}_2') \cdot \mathbf{p}_2)} |\mathbf{r}_1 \mathbf{r}_2\rangle, \tag{10.5}$$

and considering,

$$\hat{V} |\mathbf{r}_1 \mathbf{r}_2\rangle = \int V(\mathbf{r}_1', \mathbf{r}_2', \mathbf{r}_1, \mathbf{r}_2) |\mathbf{r}_1' \mathbf{r}_2'\rangle \mathrm{d}^3 r_1' \mathrm{d}^3 r_2' = \tilde{V}(\mathbf{r}_1, \mathbf{p}_1, \mathbf{r}_2, \mathbf{p}_2) |\mathbf{r}_1 \mathbf{r}_2\rangle. \tag{10.6}$$

Using the expansion over perturbations in positions, and the Fourier transform, we have transformed a general interaction depending on 4 coordinates, to depending on two coordinates with a non–locality represented by a momentum dependence.

This is a **pseudopotential**: is not strictly an interaction (being partially Fourier transformed and having a momentum dependence, and eventually other terms mimicking the many–body); is not related to the original two–body force, but is something that effectively reproduces nuclear properties (e.g. Lennard-Jones).

10.2.2 Invariance properties

To cut down the generality, we can define general symmetry properties a two–body interaction needs to have in order to have physical meaning [9, 20, 21]

- Hermiticity, $\hat{V}^+ = V$, to have real eigenvalues.
- Invariance under the exchange of coordinates, $V(1,2) = V(2,1)$, so that the interaction does not change the exchange symmetry of the wavefunction.
- Translational invariance and Rotational invariance, the system behaves equally if you change coordinates.
- Galilean invariance, in the case of non–relativistic systems the potential is not change if the system moves at constant velocity.
- Space reflection, there is no parity violation in the strong interaction.
- Time reversal, equation of motion must not depend on the time direction.

These properties can be used to bind the shape of a general interaction. For example translational and Galilean invariance means that a general two–body pseudopotential must depend only on relative coordinate $\mathbf{r}$, $\mathbf{k}$. Rotational invariance implies that the potential must be a scalar, the only three independent scalar we can construct with $\mathbf{r}$, $\mathbf{k}$ are r^2 (or more in general $v(r)$, with r scalar), p^2, and $\mathbf{r} \cdot \mathbf{k}$. However $\mathbf{k}$ changes sign under time reversal, this implies that the latter term can only appear quadratically; however $(\mathbf{r} \cdot \mathbf{k} + \mathbf{k} \cdot \mathbf{r})^2$ can be rewritten as function of r^2, p^2, L^2.

To be exchange invariant, the spin operator has to be

$$\mathbf{S} = \frac{1}{2} (\sigma_1 + \sigma_2) , \tag{10.7}$$

but since $\mathbf{S}$ has to be multiplied by a vector, also invariant under space reflection, to be a scalar. The only other operator which satisfy the requirement is $\mathbf{L}$, giving the operator part (which can be multiplied by functions of r and p) of the well known spin–orbit interaction, $\mathbf{L} \cdot \mathbf{S}$.

We have than defined a crucial structure for the central two–body interaction part of a functional generator

$$V(r) = v_0(r) + v_\sigma(r)\sigma_1 \cdot \sigma_2 + v_\tau(r)\tau_1 \cdot \tau_2 + v_{\sigma,\tau}(r)\sigma_1 \cdot \sigma_2 \tau_1 \cdot \tau_2, \tag{10.8}$$

that is more commonly written considering the spin and isospin exchange operators

$$P^\sigma = \frac{1}{2}(1 + \sigma_1 \cdot \sigma_2), \qquad P^\tau = \frac{1}{2}(1 + \tau_1 \cdot \tau_2), \tag{10.9}$$

as

$$V(r) = v_t(r) + v_x(r)P^\sigma - v_y(r)P^\tau - v_z(r)P^\sigma P^\tau, \tag{10.10}$$

From this we can define the well known families of functional generators,

10.3 Skyrme and Gogny functional generators

10.3.1 Skyrme

Skyrme interaction was proposed already in the '50 [22] as an effective contact pseudopotential, momentum dependent, with three–body contact term. After that it has evolved and taken

several different forms and parametrizations, but the most accepted being,

$$\begin{aligned}\tilde{v}^{\text{Skyrme}}(r_{12}) = \quad & t_0(1+x_0P^\sigma)\delta(\mathbf{r}_1-\mathbf{r}_2) \\ & +\tfrac{1}{2}t_1(1+x_1P^\sigma)\left[\delta(\mathbf{r}_1-\mathbf{r}_2)k'^2+k^2\delta(\mathbf{r}_1-\mathbf{r}_2)\right] && \text{Momentum Dependent} \\ & +t_2(1+x_2P^\sigma)\mathbf{k}'^*\delta(\mathbf{r}_1-\mathbf{r}_2)\cdot\mathbf{k} && \text{Momentum Dependent} \\ & +\tfrac{1}{6}t_3(1+x_3P^\sigma)\rho^\alpha(\mathbf{R})\delta(\mathbf{r}_1-\mathbf{r}_2) && \text{Density Dependent} \\ & +iW_0(\sigma_1+\sigma_2)\mathbf{k}^*\delta(\mathbf{r}_1-\mathbf{r}_2)\times\mathbf{k} && \text{Spin–Orbit}\end{aligned} \tag{10.11}$$

with $\mathbf{k}$ the relative momentum operator

$$\mathbf{k} = \frac{1}{2i}(\nabla_1 - \nabla_2). \tag{10.12}$$

$\rho^\alpha(\mathbf{R})$ is the density dependent term, usually with $1/6 \lesssim \alpha \lesssim 2/3$ and $2\mathbf{R} = \mathbf{r}_1 + \mathbf{r}_2$. In '72 Brink and Vautherin shown the equivalence of the three–body contact term with a two body, density dependent term [23] ($\alpha = 1$) in the case of time–even symmetric systems, effectively departing from the concept of interaction and introducing functional generators. Let's consider the usual definition of fields, using the distinction between isoscalar ($t = 0$, $\rho_0 = \rho_n + \rho_p$) and isovector ($t = 1$, $\rho_1 = \rho_n - \rho_p$) densities,

Time even fields

$$\rho_t(\mathbf{r},\mathbf{r}') = \sum_{i,\sigma}\psi_i^*(\mathbf{r},\sigma,\tau)\psi_i(\mathbf{r}',\sigma,\tau), \qquad \text{particle density,} \tag{10.13}$$

$$\tau_t(\mathbf{r}) = \nabla\cdot\nabla'\rho(\mathbf{r},\mathbf{r}')|_{\mathbf{r}=\mathbf{r}'}, \qquad \text{kinetic energy density,} \tag{10.14}$$

$$\mathbf{j}_t(\mathbf{r}) = \mathbf{k}\rho_t(\mathbf{r},\mathbf{r}')|_{\mathbf{r}=\mathbf{r}'}, \qquad \text{current density,} \tag{10.15}$$

Time odd fields

$$\mathbf{s}_t(\mathbf{r}) = \sum_{\sigma,\sigma'}\rho_t(\mathbf{r}\sigma,\mathbf{r}\sigma')\langle\sigma'|\hat{\boldsymbol{\sigma}}|\sigma\rangle, \qquad \text{spin density,} \tag{10.16}$$

$$\mathbf{T}_t(\mathbf{r}) = \nabla\cdot\nabla'\mathbf{s}_t(\mathbf{r},\mathbf{r}')|_{\mathbf{r}=\mathbf{r}'}, \qquad \text{spin kinetic energy density,} \tag{10.17}$$

$$\mathbb{J}_t(\mathbf{r}) = \mathbf{k}\otimes\mathbf{s}_t(\mathbf{r},\mathbf{r}')|_{\mathbf{r}=\mathbf{r}'}, \qquad \text{spin current density,} \tag{10.18}$$

where ψ_i are the Kohn-Sham wavefunctions that determine the Kohn-Sham densities.

It determines the following energy densities for the odd and even fields,

$$\mathcal{E}_t^e(\mathbf{r}) = C_t^\rho\rho_t^2 + C_t^{\Delta\rho}\rho_t\Delta\rho + C_t^\tau\rho_t\tau_t + C_t^j\mathbf{j}_t^2 + C_t^{\nabla j}\rho_t\nabla\cdot\mathbf{j}_t, \tag{10.19}$$

$$\mathcal{E}_t^o(\mathbf{r}) = C_t^s\mathbf{s}_t^2 + C_t^{\Delta s}\mathbf{s}_t\cdot\Delta\mathbf{s} + C_t^T\mathbf{s}_t\cdot\mathbf{T}_t + C_t^J\mathbb{J}_t^2 + C_t^{\nabla J}\mathbf{s}_t\nabla\times\mathbb{J}_t, \tag{10.20}$$

giving the total energy density as

$$\mathcal{E}(\mathbf{r}) = \sum_t \mathcal{E}_t^e + \mathcal{E}_t^o. \tag{10.21}$$

Where C are constants combinations of the coupling constants of the functional generator (t_i, x_i and W_0; cf. [24] for a complete and definitive list) which depends on the symmetries assumed, in particular the density depenedent term is reabsorbed in

$$C_t^\rho = C_t^\rho + C_t^{\rho DD}\rho_0^\alpha. \tag{10.22}$$

10.3.2 Coulomb

As usual, the Coulomb interaction is

$$v(r_{12}) = \frac{e^2}{4\pi\epsilon_0}\frac{1}{|\mathbf{r}_1 - \mathbf{r}_2|} \tag{10.23}$$

so its densities are given by

$$\mathcal{E}_C = \mathcal{E}_C^{dir}(\mathbf{r}) + \mathcal{E}_C^{exc}(\mathbf{r},\mathbf{r}') = \frac{e^2}{4\pi\epsilon_0}\left(\int \mathrm{d}^3r' \frac{\rho(\mathbf{r}_p\rho(\mathbf{r}'_p}{|\mathbf{r}-\mathbf{r}'|} - \frac{\rho_p^2(\mathbf{r},\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|}\right) \tag{10.24}$$

where the direct energy density considers the charge density as the proton one, while the exchange term would require the employment of the non–local density $\rho(\mathbf{r},\mathbf{r}') = \sum_i \psi_i^*(\mathbf{r}\sigma q)\psi_i(\mathbf{r}'\sigma q)$, to be solved exactly.

An approximation to reduce this non–local exchange term to a local functional is the Slater approximation [25]

$$-\frac{e^2}{4\pi\epsilon_0}\frac{\rho_p^2(\mathbf{r},\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|} \approx -\frac{3e^2}{8\epsilon_0}\left(\frac{3}{\pi}\right)^{\frac{1}{3}}\rho_p^{4/3}(\mathbf{r}) \tag{10.25}$$

10.3.3 Gogny

Gogny and Dechargé, [26] have introduced in 1980 a finite–range functional based on a sum of two gaussians, with the usual zero range density dependence and spin–orbit, Gogny D1, that has proven to be very successful (especially the new readjustments D1S and D1M),

$$\begin{array}{lll} \tilde{v}^{\mathrm{Gogny}}(r_{12}) = \sum_j^{2(3)} = 1 & e^{-(\mathbf{r}_1-\mathbf{r}_2)^2/\mu_j^2}(W_j + B_jP^\sigma - H_jP^\tau - M_jP^\sigma P^\tau) & \text{sum of Gaussians,} \\ & +t_3(1+x_3P^\sigma)\rho^\alpha(\mathbf{R})\delta(\mathbf{r}_1-\mathbf{r}_2) & \text{Density Dependent,} \\ & +iW_0(\sigma_1+\sigma_2)\mathbf{k}^*\delta(\mathbf{r}_1-\mathbf{r}_2)\times\mathbf{k} & \text{Spin–Orbit.} \end{array} \tag{10.26}$$

10.4 BCP functional

The Barcellona–Catania–Paris [27] is a good example of a pure Kohn-Sham scheme functional in nuclear physics. Defines the energy from the following ansatz

$$E = T_0 + E^{s.o.} + E_{int}^{FR} + E_{int}^{\infty} + E_C \tag{10.27}$$

with T_0 the kinetic term, $E^{s.o.}$ the spin orbit (uncorrelated), E_{int} the proper nuclear interaction part, split in a Finite–Range (FR) and a bulk (∞) term, and E_C the Coulomb contribution

respectively. More precisely,

$$T_0 = \frac{\hbar^2}{2m} \sum_{\sigma,q} \int \mathrm{d}^3 r \tau_q(\mathbf{r}, \sigma, \mathbf{q}) \tag{10.28}$$

$$E_C[\rho_p] = \frac{1}{2} \int \mathrm{d}^3 r \mathrm{d}^3 r' \frac{\rho_p(\mathbf{r})\rho_p(\mathbf{r}')}{\mathbf{r} - \mathbf{r}'} - \frac{3}{4} \left(\frac{3}{\pi}\right)^{\frac{1}{3}} \int \mathrm{d}^3 r \rho_p^{4/3}(\mathbf{r}) \tag{10.29}$$

$$E_{int}^{FR}[\rho_n, \rho_p] = \frac{1}{2} \sum_{q,q'} \int \mathrm{d}^3 r \mathrm{d}^3 r' \rho_t(\mathbf{r}) v_{q,q'}(\mathbf{r} - \mathbf{r}') \rho_{q'}(\mathbf{r}') - \frac{1}{2} \sum_{q,q'} \int \mathrm{d}^3 r \rho_q(\mathbf{r}) \rho_{q'}(\mathbf{r}) v_{q,q'} \int \mathrm{d}^3 r' v_{q,q'}(\mathbf{r}') \tag{10.30}$$

$$E_{int}^{\infty}[\rho_n, \rho_p] = \int \mathrm{d}^3 r \left[P_s(\rho) \left(1 - \beta^2\right) + P_n(\rho) \beta^2 \right] \rho \tag{10.31}$$

where $v_{q,q'}(\mathbf{r}')$ is a central Gaussian, $\rho = \rho_p + \rho_n$, $\beta\rho = \rho_p - \rho_n$, P_s and P_n are polynomials (to the fifth power) of ρ. The resulting functional is now non–local.

10.5 Exercise

Exercise 41.

Calculate the energy density corresponding to a free (non interacting $v(r_{12}) = 0$) fermion gas in spherical symmetry, remembering that wavefunction for the free system are plane waves

$$\psi(\mathbf{r}) = \frac{1}{(2\pi)^{3/2}} e^{i\mathbf{r}\cdot\mathbf{k}} \tag{10.32}$$

Exercise 42.

Calculate the energy density corresponding to the central term of Gogny functional generator

$$v^{\text{Gogny}}(r_{12}) = \sum_{j}^{2(3)} = 1\ e^{-(\mathbf{r}_1-\mathbf{r}_2)^2/\mu_j^2}(W_j + B_j P^\sigma - H_j P^\tau - M_j P^\sigma P^\tau) \tag{10.33}$$

Exercise 43.

Considering that the Galilean invariance implies on the functional that

$$\rho(\mathbf{x}, \mathbf{x}') = e^{\frac{i}{\hbar}\mathbf{P}\cdot(\mathbf{r}-\mathbf{r}')}\rho'(\mathbf{x}, \mathbf{x}'), \tag{10.34}$$

Demonstrate that the term $\rho\tau - j^2$ is Galilean invariant.

Lecture 11

Lecture 11: Phenomenological nuclear functionals II [Week 3, day 1]

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11.1 SelfInteraction

If we consider Coulomb functional in the Slater approximation

$$\mathcal{E}_C(\mathbf{r}) = \frac{e^2}{4\pi\epsilon_0}\left(\int \frac{\rho_p(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|} - \frac{3}{2}\left(\frac{3}{\pi}\right)^{\frac{1}{3}}\rho_p^{1/3}(\mathbf{r})\right)\rho_p(\mathbf{r}) \neq 0, \tag{11.1}$$

for one particle $\rho(\mathbf{r}) = |\psi_0(\mathbf{r})|^2$, and this should be zero but it is not! However the original non–local functiontal exactly derived from the interaction it is,

$$\frac{e^2}{4\pi\epsilon_0}\left(\int \mathrm{d}^3r' \frac{\rho_p(\mathbf{r})\rho_p(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|} - \frac{\rho_p^2(\mathbf{r},\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|}\right) = 0, \tag{11.2}$$

that for one particle is $\rho(\mathbf{r},\mathbf{r}') = \psi_0^*(\mathbf{r}')\psi_0(\mathbf{r})$

So, first of all, beware on the conditions that have to be satisfied by your functional. Second of all consider that the functional form, that is not derived exactly from an interaction form, contains implicitly self–interaction terms. This self–interaction terms make going beyond the mean field level very difficult, e.g. generating instabilities when projecting.

11.2 Nuclear Matter properties

For a time–even system, I can write the Hamiltonian density as

$$\mathcal{H}(\mathbf{r}) = \frac{\hbar^2}{2m}\tau_t + C_t^\rho \rho_t^2 + C_t^{\Delta\rho}\rho_t\Delta\rho + C_t^\tau \rho_t\tau_t + C_t^j \mathbf{j}_t^2 + C_t^{\nabla j}\rho_t\nabla\cdot\mathbf{j}_t, \tag{11.3}$$

and the relation between densitis and Fermi momentum in the free Fermi gas is

$$\rho = \frac{2}{3\pi^2}k_F^3; \qquad \tau = \frac{3}{5}\left(\frac{3\pi^2}{2}\right)^{2/3}\rho^{5/3}. \tag{11.4}$$

Because of translational invariance in infinite matter $\nabla\rho = \nabla\cdot\mathbf{j} = 0$, and if the matter is spin-saturated I don't have the spin orbit density $\mathbf{j}_t = 0$.

Binding Energy per particle is given by,

$$\frac{E_0}{A} = \frac{\mathcal{H}}{\rho} = \frac{3\hbar^2}{10m}k_F^2 + C_t^\rho\rho + \frac{3}{5}C_t^\tau\rho k_F^2, \tag{11.5}$$

binding energy per particle in function of ρ is called Equation of State and contains the information regarding the static and dynamic properties of infinite nuclear matter.

and I can try to look for a minimum in the binding energy per particle that my functional gives, which is an equilibrium density ρ_0 called *saturation density*

$$\left.\frac{\delta E_0/A}{\delta\rho}\right|_{\rho=\rho_0} = \left.\frac{3\hbar^2}{10m}k_F^2\rho^{-1} + C_t^\rho + \frac{3}{5}C_t^\tau k_F^2\right|_{\rho=\rho_0} = 0. \tag{11.6}$$

Incompressiblity K is the curvature of the equation of state around the saturation density respect to the Fermi momentum,

$$K = k_F^2\left.\frac{\partial^2(E_0/A)}{\partial k_F^2}\right|_{\rho=\rho_0} = \frac{6\hbar^2}{10m}k_F^2 + 6\tilde{C}_t^\rho\rho + \frac{60}{5}C_t^\tau\rho k_F^2 \tag{11.7}$$

11.2.0.1 Effective mass

It is convenient to collect $C_t^\tau\rho_t\tau_t$ with the kinetic term, defining an *effective mass* which includes some non–local (velocity dependent) terms of the functional

$$m_k(\mathbf{r}) := m\left(1 + \frac{2m}{\hbar^2}C_t^\tau\rho_t\right)^{-1} = \frac{\hbar^2}{2}\left(\frac{\delta\mathcal{H}}{\delta\tau}\right)^{-1} \tag{11.8}$$

11.3 Experimental and other constraints

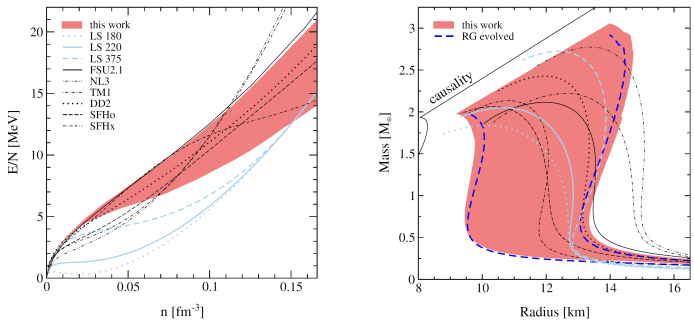

Figure 11.1: Chiral–EFT contraints on pure neutron matter Equation Of State (left) and neutron–star mass–radius relation [28].

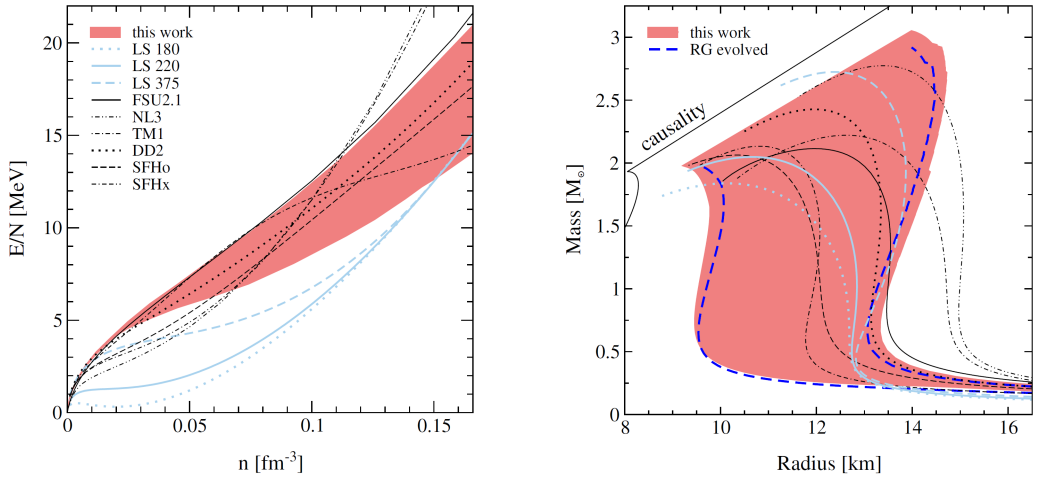

Figure 11.2: Chiral–EFT contraints on pure neutron matter Equation Of State (left) and neutron–star mass–radius relation [28].

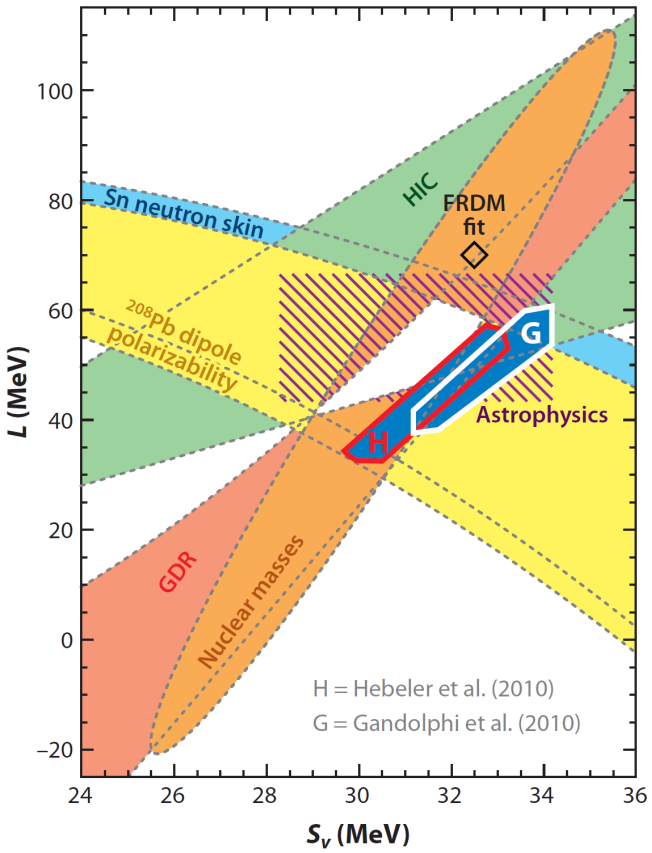

Figure 11.3: Summary of constraints on symmetry energy parameters. The filled ellipsoid indicates joint $S_v L$, with S_v symmetry energy and L the density independent part of the symmetry energy, are constrained by nuclear masses [29]. The finite-range droplet model fit [30] is indicated with a diamond. The filled bands show constraints from neutron skin thickness of tin (Sn) isotopes [31], isotope diffusion in heavy-ion collisions (HIC), the dipole polarizability of 208Pb [32], and giant dipole resonances (GDR) [33]. The hatched rectangle shows constraints from astrophysical modeling of Masses–Radii observations. The two closed curves show neutron matter constraints (H is from [34], and G is from [35].) The white area is the experimentally allowed overlap region. cf. [36].

	BCP1	D1S	SLy4
rms_E [MeV]	1.775	2.414	1.711
rms_R [fm]	0.031	0.020	0.024

Table 11.1: RMS deviations of energies and radii given in [27].

11.4 Performance of common functionals

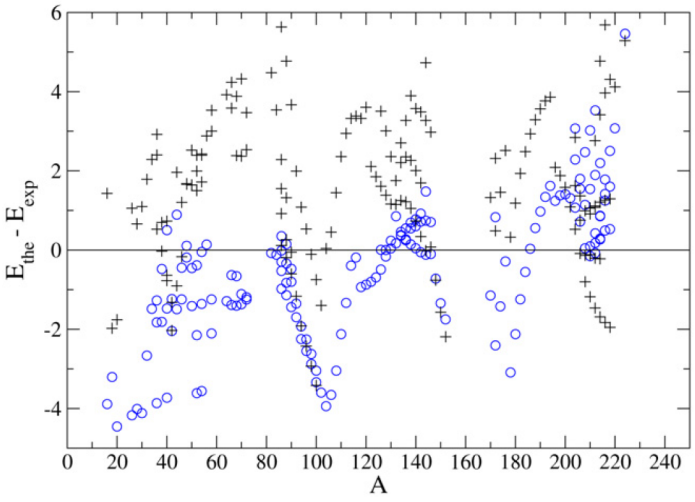

Figure 11.4: Comparison between BCP (dots) and D1S (crosses) functionals [27].

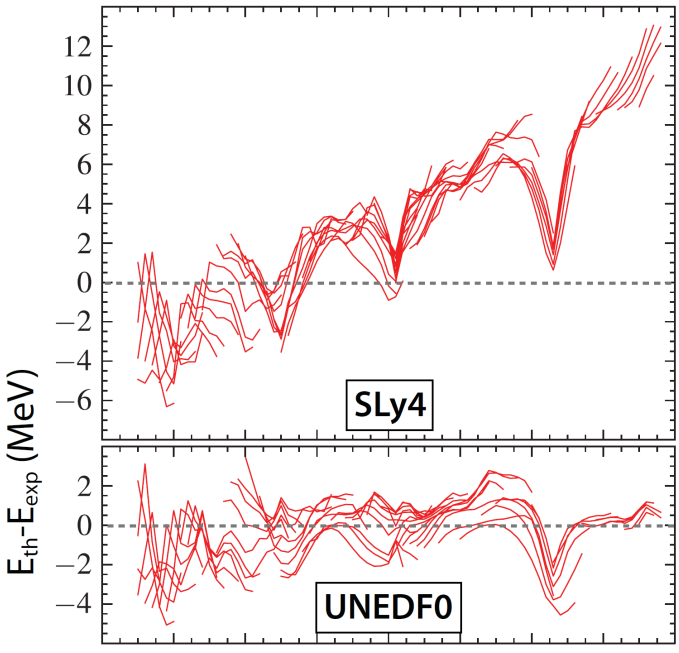

Figure 11.5: Comparison between two different fits of the same Skyrme functional form, one is fitted in a way more sophisticated way [29].

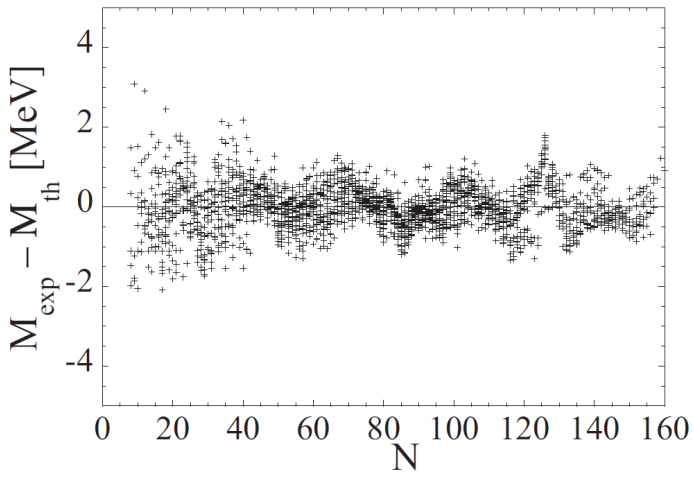

Figure 11.6: A very rich functional, constantly updated and further corrected for beyond–mean–field correlations, still not that much better [37].

11.5 Pairing forces

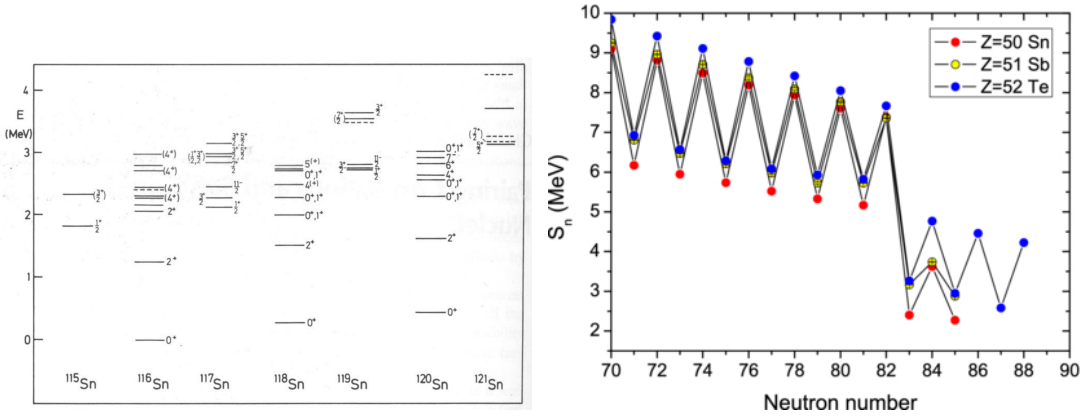

Figure 11.7: Excited states spectrum of even an odd Sn isotopes [9] (left) and example of odd–even mass staggering represented in the neutron separation energy for neutron rich isotopes of Sn, Sb and Te [38] (right).

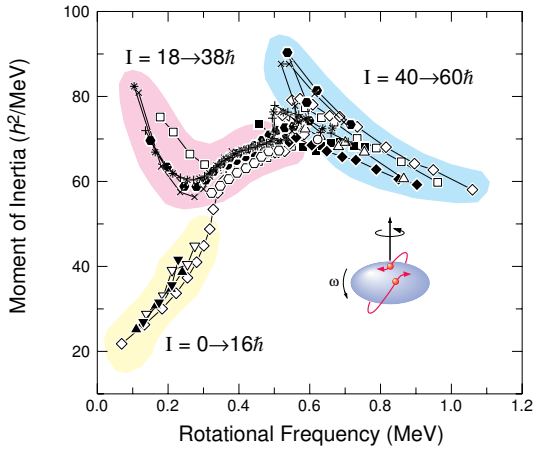

Figure 11.8: Textbook example of backbanding due to pair breaking ^{156}Dy [39] (right).

There are several ways to introduce pairing into a functional, again phenomenological guidance is paramount. Ideally one would like consistency within the functional in the particle–hole and particle–particle channel, but only Gogny and very few of the Skyrme functionals are able to deliver sensible pairing properties.

For this reason pairing is often "attached" in various forms that not necessarly have the same form of the functional in the particle–hole channel.

Phenomenologically even in the '50 Maria Göppelt–Mayer realized that a short range interaction between nucleons in $J = 0$ states could explain odd-even staggering [40].

11.5.1 Seniority Pairing

The seniority scheme is the quintessential pairing interaction

$$\hat{V}_p^{sen} = -G\hat{P}_m^+\hat{P}_{m'} = -G\sum_{m,m'>0} a_m^+ a_{\bar{m}}^+ a_{\bar{m}'} a_{m'}, \tag{11.9}$$

where $\hat{P}_m^+$, $\hat{P}_m$ are pair creation and annihilation operators and create or destroy pair of particles in time reversal. The interaction can be rewritten to be $V_p^{sen} \approx -\Delta(P^+ + P) + \Delta^2/G$, by omitting $(P^+ - < P >)(P - < P >)$ considering small variations around the ground states, where $\Delta := G\langle BCS|P|BCS\rangle$.

I recall that the BCS ansatz vacuum is defined as $|BCS\rangle = \prod_{m>0}(U_m V_m a_m a_{\bar{m}}^{\pm})|0\rangle$, however here I haven't used the notion and I could define the BCS vacuum starting from the seniority pairing operator. Since the average value of the $\langle BCS|\hat{N}|BCS\rangle = 2\sum_{m>0} V_m^2 = N$ in the BCS ground state is not fixed, I have to constrain my single–particle Hamiltonian with a Lagrange multiplier λ that imposes the number of particles N.

This gives a total mean field + pairing hamiltonian

$$H = H_{sp} - \lambda\hat{N} + V_p = \sum_{m>0}(\varepsilon_m - \lambda)(a_{\bar{m}}^+ a_{\bar{m}} a_m^+ a_m) - \Delta(a_m^+ a_{\bar{m}}^+ + a_{\bar{m}} a_m) + \Delta^2/G, \tag{11.10}$$

which is bilinear in creation operator. To solve it make use of the usual techniques I need to rotate the a^+, a space, making use of the Bogoliubov–Valatin transformation (cf. Lecture 6, Sect. 6.2.1),

$$\begin{array}{ll} \alpha_m^\dagger = U_m a_m^\dagger + V_{\bar{m}} c_{\bar{m}}, & \alpha_m = U_m^* a_m + V_{\bar{m}}^* a_{\bar{m}}^\dagger, \\ \alpha_{\bar{m}}^\dagger = U_{\bar{m}} a_{\bar{m}}^\dagger + V_m c_m, & \alpha_{\bar{m}} = U_{\bar{m}}^* a_{\bar{m}} + v_m^* a_m^\dagger, \end{array}, \tag{11.11}$$

that enable to rewrite the hamiltonian in the *quasiparticle basis*,

$$H = \sum_{m>0} E_m(\alpha_m^+\alpha_m + \alpha_{\bar{m}}^+\alpha_{\bar{m}}) + const. \tag{11.12}$$

By equating Eq. (11.10) and (11.12), and representing the bilinear forms as off–diagonal matrix elements ones get

$$E_m \begin{pmatrix} U_m \\ V_m \end{pmatrix} = \begin{pmatrix} \varepsilon_m - \lambda & \Delta \\ \Delta & \varepsilon_m - \lambda \end{pmatrix} \begin{pmatrix} U_m \\ V_m \end{pmatrix}, \tag{11.13}$$

which eigenvalue and eigenvector solution define the properties of the BCS quasiparticles

$$E_m = \sqrt{(\varepsilon_m - \lambda) + \Delta^2}\,; \qquad \left.\begin{matrix} U_m^2 \\ V_m^2 \end{matrix}\right\} = \frac{1}{2}\left(1 \pm \frac{\varepsilon_m - \lambda}{E_m}\right), \tag{11.14}$$

together with the fact that we want the Bogoliubov transformation to be unitary, so

$$\{\alpha_m, \alpha_{m'}\} := \delta_{m,m'} \Rightarrow U_m^2 + V_m^2 = 1. \tag{11.15}$$

To be noted that Eq. 11.13 and following are still valid for a more general interaction $v_{m\bar{m}m'\bar{m}'}$ once adopting a state–dependent pairing gap Δ_m.

λ and Δ deserve a talk in their own right: λ defines the Hamiltonian H' above setting the number of particles of the system we want to describe as a Lagrange multiplier, this is solved consistently within the definition of V_m in what is called *number equation*,

$$N = 2\sum_{m>0} V_m^2. \tag{11.16}$$

Δ is the pairing gap, which is related to the average value of $\hat{P}$ operator, $\alpha_0 = \langle BCS|P^+|BCS\rangle = \sum_{m>0} U_m V_m$, that substituting with Eq. (11.14) and eventually for a general BCS–type pairing interaction,

$$\Delta_m = -\sum_{m'>0} v_{m\bar{m}m'\bar{m}'} U_{m'} V_{m'} = -\frac{1}{2}\sum_{m'>0} \frac{\Delta_{m'}}{(\varepsilon_{m'}-\lambda)^2 + \Delta_{m'}^2} \tag{11.17}$$

is known as *Gap Equation*. Solving iteratively Number, Gap Equations and making use of eigenvalue Eqs. (11.13) we get BCS solutions of the system, used to describe fermion superfluidity.

This which has extremely interesting physical properties concerning nuclear superfluidity, being studied and reflected in virtually every nuclear observable such as odd-even mass differences, particle–hole occupation factors, excitation energy of single particle and collective states, 2–particle transfer reactions, rotation inertia ...etc...

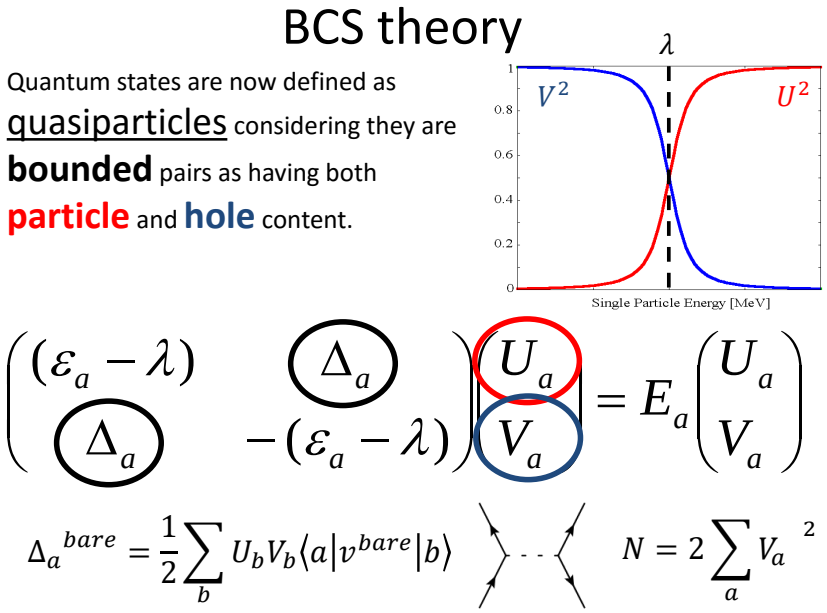

Figure 11.9:

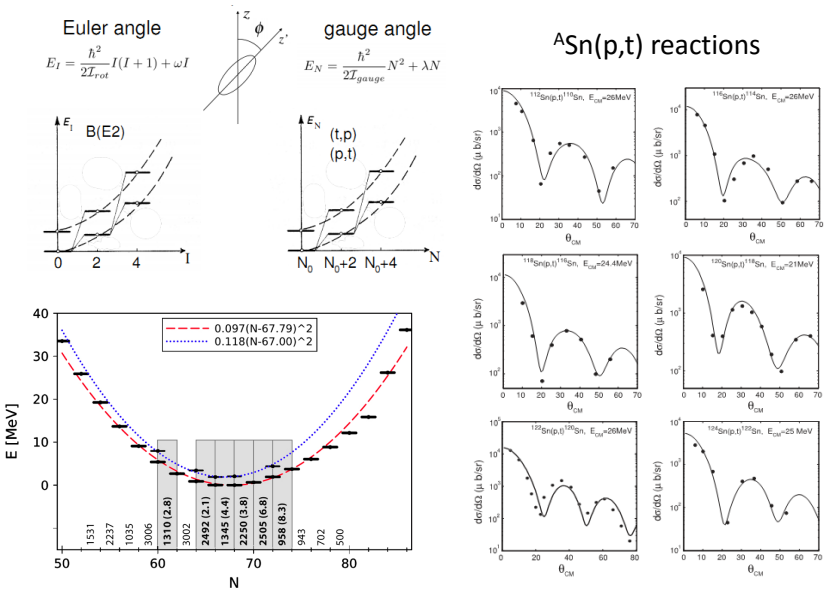

Figure 11.10: cf. [41],[42]

11.5.2 Pairing Functional

A simple delta pairing interaction $v(r_{12}) = t'_0(1 + x'_0 P^\sigma)\delta(\mathbf{r}_1 - \mathbf{r}_2)$, generates a similar (but not equal) functional in the pairing channel, as it does in the particle–hole,

$$\mathcal{E}^{pair} = \frac{t'_0}{4}(1 - x'_0)(\rho_n^2 + \rho_p^2) \tag{11.18}$$

To derivate it we have to consider the nature of densities in the pairing channel. If in the particle–hole channel, densities can be written as

$$\hat{\rho}(\mathbf{r}_1 s_1 t_1, \mathbf{r}_2 s_2 t_2) = \langle \Psi | a^\dagger_{\mathbf{r}_2 s_2 t_2} a_{\mathbf{r}_1 s_1 t_1} | \Psi \rangle \,, \tag{11.19}$$

which eventually gives, in the general case with isospin mixing,

$$\begin{aligned}\hat{\rho}(\mathbf{r}_1 s_1 t_1, \mathbf{r}_2 s_2 t_2) = \frac{1}{4}(&\rho_0(\mathbf{r}_1, \mathbf{r}_2)\delta_{s_1 s_2}\delta_{t_1 t_2} + \rho_1(\mathbf{r}_1, \mathbf{r}_2)\delta_{s_1 s_2}\hat{\tau}^{(3)}_{t_1 t_2} \\ &+ \mathbf{s}_0(\mathbf{r}_1, \mathbf{r}_2)\cdot\hat{\boldsymbol{\sigma}}_{s_1 s_2}\delta_{t_1 t_2} + \mathbf{s}_1(\mathbf{r}_1, \mathbf{r}_2)\cdot\hat{\boldsymbol{\sigma}}_{s_1 s_2}\hat{\tau}^{(3)}_{t_1 t_2}).\end{aligned} \tag{11.20}$$

However, in the particle–particle channel densities arise from the application of two creation or destruction operator from the fact that the ground state is not anymore annihilated by bilinear operators,

$$\hat{\tilde{\rho}}(\mathbf{r}_1 s_1 t_1, \mathbf{r}_2 s_2 t_2) = -2 s_2 \langle \Psi | a_{\mathbf{r}_2 \text{-} s_2 t_2} a_{\mathbf{r}_1 s_1 t_1} | \Psi \rangle \,, \tag{11.21}$$

bringing a different relation and different symmetries,

$$\hat{\rho}(\mathbf{r}_1 s_1 t_1, \mathbf{r}_2 s_2 t_2) = \hat{\rho}^*(\mathbf{r}_2 s_2 t_2, \mathbf{r}_1 s_1 t_1) \,, \tag{11.22}$$

$$\hat{\tilde{\rho}}(\mathbf{r}_1 s_1 t_1, \mathbf{r}_2 s_2 t_2) = 4 s_1 s_2 \,\hat{\tilde{\rho}}(\mathbf{r}_2 \text{-} s_2 t_2, \mathbf{r}_1 \text{-} s_1 t_1) \,, \tag{11.23}$$

and while the densities are subdivided in the same way (scalar, spin, eventually, but not in this case, isospin)

$$\hat{\tilde{\rho}}_t(\mathbf{r}_1 s_1, \mathbf{r}_2 s_2) = \frac{1}{2}(\tilde{\rho}_t(\mathbf{r}_1, \mathbf{r}_2)\delta_{s_1 s_2} + \tilde{\mathbf{s}}_t(\mathbf{r}_1, \mathbf{r}_2)\cdot\hat{\boldsymbol{\sigma}}_{s_1 s_2}) \,, \tag{11.24}$$

the decomposition of the spin exchange operators in the particle–particle are not the same as in the particle–hole, since the bilinear operators recouple all the indexes,

$$4\sigma'_2\sigma_2 P^\sigma_{\sigma'_1 - \sigma'_2 \sigma'_2 - \sigma_2} = \frac{1}{2}\left(-\delta_{\sigma'_2\sigma'_1\sigma_2\sigma_1} + \hat{\sigma}_{\sigma'_2\sigma'_1}\cdot\sigma_{\sigma_2\sigma_1}\right). \tag{11.25}$$

Tackling directly this form of the exchange operator can be tricky, thus one of the most practical way to derive the pairing functional is by considering the aforementioned symmetry properties of the densities in the particle–particle channel and considering that the action of the spin exchange operator on the density is

$$\sum_{s_1, s_2} \tilde{\rho}^*(\mathbf{r}_1 s_1, \mathbf{r}_2 s_2)\tilde{\rho}(\mathbf{r}_1 s_2, \mathbf{r}_2 s_1) = \frac{1}{2}[-\rho\tilde{\rho}(\mathbf{r}_1 s_1, \mathbf{r}_2 s_2)\tilde{\rho}^*(\mathbf{r}_1, \mathbf{r}_2)\tilde{\rho}^*(\mathbf{r}_1, \mathbf{r}_2) - \tilde{\mathbf{s}}^*(\mathbf{r}_1, \mathbf{r}_2)\cdot\mathbf{s}(\mathbf{r}_1, \mathbf{r}_2)], \tag{11.26}$$

that is -1/2 on scalar density and +1/2 on spin density. Giving the final energy density as

$$\tilde{\mathcal{E}} = \frac{t'_0}{4}(1 - x'_0)\tilde{\rho}^2(\mathbf{r}) + \frac{t'_0}{4}(1 + x'_0)\tilde{\mathbf{s}}^2(\mathbf{r}) \tag{11.27}$$

11.5.3 Surface–Volume

In practical calculations the standard is often considered to be the above calculated local and zero-range [43], however there is a further sophistication that can be employed that is the introduction of a form factor that with the density dependence emulates a surface surface or volume predominance of the pairing interaction:

$$\hat{V}_{\text{pair}}(\mathbf{r}_1, \mathbf{r}_2) = \sum_{t=n,p} V_t \left(1 - \alpha \frac{\rho(\mathbf{R})}{\rho_0}\right) \delta(\mathbf{r}_1 - \mathbf{r}_2), \tag{11.28}$$

with $\mathbf{R} = (\mathbf{r}_1 + \mathbf{r}_2)/2$, $\rho_0 = 0.16$ fm^{-3} is the saturation density. If $\alpha = 1$, we have a *surface* pairing force, if $\alpha = 0$ we have a *volume* pairing force; often, $\alpha = 1/2$.

11.6 Exercise

Read a lot of the provided literature.

Lecture 12

Nuclear phenomenology

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12.1 Nilsson orbitals

A very valid alternative to describe properties of nuclei is represented by phenomenological potentials. In Fig.12.3 some simple phenomenological potentials for a schematic 1D case.

The potential that resembles the most the result of an HF calculation is the Wood-Saxon.

$$V^{WS}(r) = V_0 \left[1 + \exp\left(\frac{r - R_0}{a}\right)\right]^{-1} \tag{12.1}$$

the problem of this potential (see computational class) is that it is very difficult to find analytical solutions and one need to solve it numerically. An alternative is to use the HO potential. For the case of no spin-orbit the solutions are known analytically. We follow here the derivation of Nilsson.

We consider the phenomenological Hamiltonian to describe nuclear properties

$$H = -\frac{\hbar^2}{2M}\Delta + \frac{1}{2}M\omega_0^2 r^2 - C\,\boldsymbol{l}\cdot\boldsymbol{s} - D\left(l^2 - \langle l^2\rangle_N\right) \tag{12.2}$$

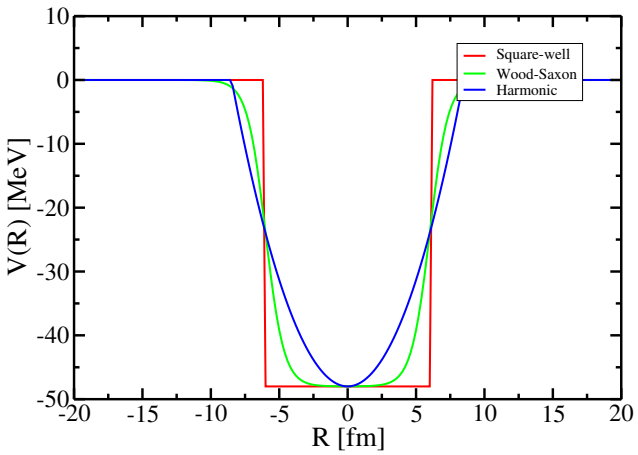

Figure 12.1: Phenomenological potentials.

the ;$\boldsymbol{l}\cdot\boldsymbol{s}$ spin orbit term has been added to reproduce magic numbers. The term l^2 has been added to reproduce the mode accurate Wood-Saxon potential. While $\langle l^2\rangle_N = N(N+3)/2$ has been added to avoid too much compression of the shells due to l^2.

We can easily apply it to the deformed case (assume axial symmetry along z)

$$H = -\frac{\hbar^2}{2M}\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}\right)+\frac{M}{2}\left[\omega_\perp^2(x^2+y^2)+\omega_z^2 z^2\right]-C\,\boldsymbol{l}\cdot\boldsymbol{s}-D(l^2-\langle l^2\rangle_N) \quad (12.3)$$

where

$$\omega_z = \omega_0\left(1-\frac{2}{3}\varepsilon\right) \quad (12.4)$$

$$\omega_\perp = \omega_0\left(1+\frac{1}{3}\varepsilon\right) \quad (12.5)$$

the distorsion parameter ε is defined as $\varepsilon = (\omega_\perp - \omega_z)/\omega_0$. For $\varepsilon > 0$ (< 0) we have prolate (oblate) shapes. The problem can be solved in the two extreme cases: very small and very large deformation

12.1.1 small ε

We consider very small deformation so that we can write the hamiltonian as $H_0^{sph} + \varepsilon h'$ that reads

$$\varepsilon h' = \varepsilon\frac{M}{2}\frac{2}{3}\omega_0^2(x^2+y^2-2z^2) = -\frac{M}{2}\omega_0^2\frac{4}{3}\varepsilon r^2 P_2(\cos\theta) \quad (12.6)$$

the eigenfunction of a pure spherical case would read

$$\phi(Nlsj\Omega) = R_{Nl}(r)\sum_{\Lambda\Sigma} C^{j\Omega}_{l\Lambda\frac{1}{2}\Sigma} Y_{l\Lambda}(\hat{r})\chi_{\frac{1}{2}\Sigma} \tag{12.7}$$

here $\boldsymbol{j} = \boldsymbol{l} + \boldsymbol{s}$ and Ω is the z-axis projection of j. In the spherical case each state is (2j+1)-fold degenerate. This degeneracy is removed by the small perturbation that we can calculate at first order as

$$\langle Nlsj\Omega|\varepsilon h'|Nlsj\Omega\rangle = \frac{1}{6}\varepsilon M\omega_0^2\langle r^2\rangle\frac{3\Omega^2 - j(j+1)}{j(j+1)} \tag{12.8}$$

(See exercise). We see that the states with $\Omega < j$ move down in energy and thus they are favoured compared to states with $\Omega \approx j$ that get a much smaller contribution. For oblate deformation the opposite is true.

12.1.2 very large ε

We now consider very large deformations we can consider the corrective terms l^2 and $l \cdot s$ as perturbations.

We thus split H into $H_{osc} + h'$ where

$$H_{osc} = -\frac{\hbar^2}{2M}\Delta + \frac{M}{2}\left[\omega_\perp^2(x^2+y^2) + \omega_z^2 z^2\right] \tag{12.9}$$

Where h' contain terms that play a minor role as l^2 or $l \cdot s$ We introduce *stretched* coordinates as

$$\chi = x\left(\frac{M\omega_\perp}{\hbar}\right)^{1/2}, \eta = y\left(\frac{M\omega_\perp}{\hbar}\right)^{1/2}, \xi = z\left(\frac{M\omega_z}{\hbar}\right)^{1/2} \tag{12.10}$$

so we can rewrite H as

$$H_{osc} = \frac{1}{2}\hbar\omega_\perp\left[-\left(\frac{\partial^2}{\partial\chi^2} + \frac{\partial^2}{\partial\eta^2} + (\chi^2+\eta^2)\right)\right] + \frac{1}{2}\hbar\omega_z\left(-\frac{\partial^2}{\partial\xi^2} + \xi^2\right) \tag{12.11}$$

We no go to cylindrical coordinates (ρ, ϕ, ξ) where

$$\chi = \rho\cos\phi \tag{12.12}$$
$$\eta = \rho\sin\phi \tag{12.13}$$

We can write the Schroedinger equation as

$$\left[\frac{1}{2}\hbar\omega_\perp\left(-\frac{1}{\rho}\frac{\partial}{\partial\rho}\rho\frac{\partial}{\partial\rho}-\frac{1}{\rho^2}\frac{\partial^2}{\partial\phi^2}+\rho^2\right)+\frac{1}{2}\hbar\omega_z\left(-\frac{\partial^2}{\partial\xi^2}+\xi^2\right)-E\right]=0 \tag{12.14}$$

We now separate the ϕ part by assuming our solution to be $\psi = U(\rho)Z(\xi)\Phi(\phi)$. We have

$$-\frac{\partial^2}{\partial\phi^2}\Phi=\Lambda\phi \tag{12.15}$$

with solution $\Phi = e^{i\Lambda\phi}$. This is the consequence of $[L_z, H] = 0$ and $L_z = \Lambda$ is a constant of motion. For the ξ part we get

$$\hbar\omega_z\left(-\frac{\partial^2}{\partial\xi^2}+\xi^2\right)Z(\xi)=E_zZ(\xi) \tag{12.16}$$

this is 1-D HO equation $E_z = \hbar\omega_z(n_z + 1/2)$. And $E = E_\perp + E_z$.

$$\frac{1}{2}\hbar\omega_\perp\left(-\frac{1}{\rho}\frac{\partial}{\partial\rho}\rho\frac{\partial}{\partial\rho}+\frac{\Lambda^2}{\rho^2}+\rho^2\right)U(\rho)=E_\perp U(\rho) \tag{12.17}$$

We assume a solution form $U = \rho^{|\Lambda|}e^{-\rho^2/2}W(\rho)$, so replacing in previous equation we get for W

$$zW''+(|\Lambda|+1-z)W'-\frac{1}{2}\left(|\Lambda|+1-\frac{E_\perp}{\hbar\omega_\perp}\right)W=0 \tag{12.18}$$

where $z = \rho^2$. The solution of this equation is called hypergeometric function

$$W=F\left(\frac{1}{2}(|\Lambda|+1-\frac{E_\perp}{\hbar\omega_\perp}),|\Lambda|+1;z\right) \tag{12.19}$$

with $E_\perp = \hbar\omega_\perp(2n_p + |\Lambda| + 1) = \hbar\omega_\perp(n_\perp + 1)$.

We can now summarise the results as

$$E=\hbar\omega_z\left(n_z+\frac{1}{2}\right)+\hbar\omega_\perp(n_\perp+1)=\hbar\omega_0\left(N+\frac{3}{2}+\frac{\epsilon}{3}(n_\perp-2n_z)\right) \tag{12.20}$$

$$\Psi=Ce^{-\xi^2/2}H_{n_z}(\xi)\rho^{|\Lambda|}e^{-\rho^2/2}F\left(-\frac{n_\perp-|\Lambda|}{2},|\Lambda|+1;\rho^2\right)e^{i\Lambda\phi} \tag{12.21}$$

We notice that we have a shell structure at $\epsilon = 0; 0.6; 1, -0.75$. On top of this we need now to calculate the correction induced by the other term we have left apart. We can calculate them as a perturbation

$$\langle N n_z \Lambda\Sigma | l \cdot s | N n_z \Lambda\Sigma \rangle = \Lambda\Sigma \tag{12.22}$$

$$\langle N n_z \Lambda\Sigma | l^2 | N n_z \Lambda\Sigma \rangle = \Lambda^2 + 2n_\perp + n_z + 2n_z + n_\perp \tag{12.23}$$

The effect of the inclusion of these terms is to remove the $2 \times (n_\perp + 1)$-fold degeneracy and only a two fold (Kramer) degeneracy is left (time reversal conserving).

In the intermediate region these approximations do not hold anymore and we have to solve the problem numerically. We can expand the problem over the basis $|Nl\Lambda\Sigma$, but now $[j_z, H] = 0$. So we have $\Omega = \Lambda + \Sigma$

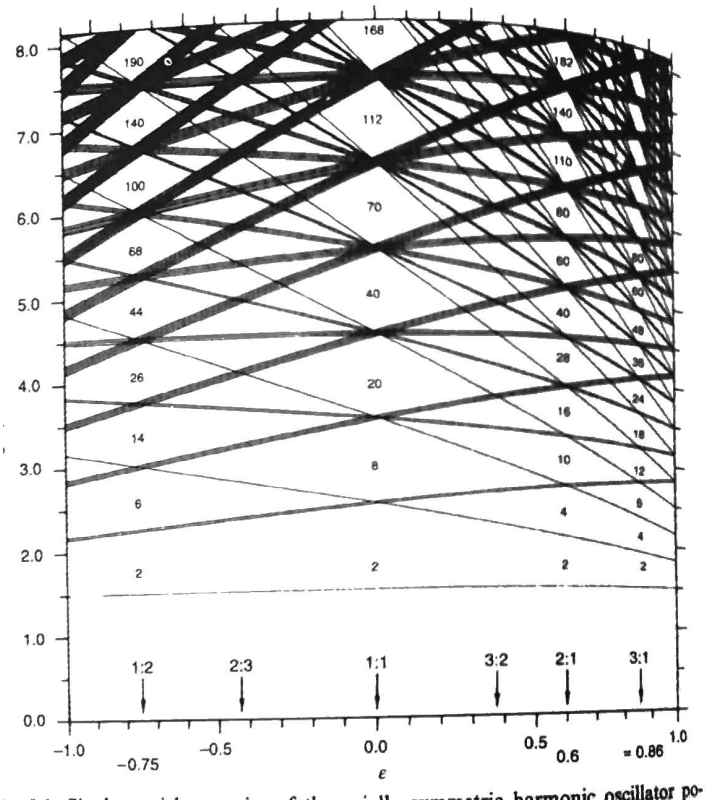

Figure 12.2: Nilsson orbitals in the limit of very large deformations. Taken from [44].

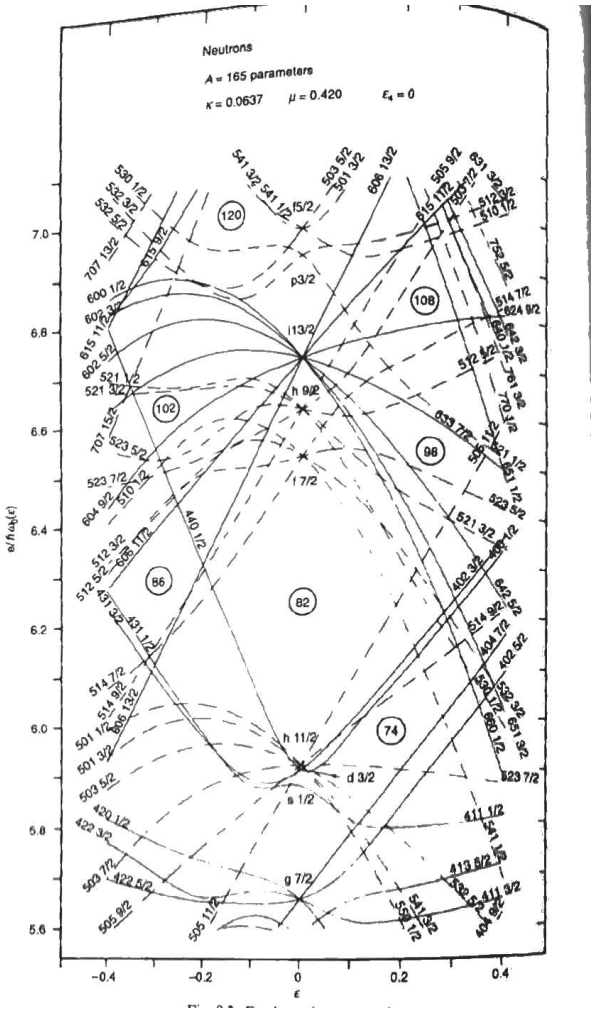

Figure 12.3: Nilsson orbitals. Complete calculation. Taken from [44].

12.2 Particle rotor-model

Rotation is a typical example of collective motion.By looking at occurrence of rotational bands one could determine if the nucleus is deformed or not. In practice pure rotational bands are never realised.

$$E_I = \frac{\hbar^2}{2\mathcal{I}} I(I+1) \tag{12.24}$$

If exact the ratio $E(I=4) : E(I=2) = 3.33$, only in few nuclear system this is *almost* the case: rare earth region. We assume that the Hamiltonian can be written as $H = H_{int} + H_{coll}$. The intrinsic part is

$$H_{int} = \sum_k e_k a_k^\dagger a_k + \frac{1}{4} \sum_{klmn} \bar{v}_{klmn} a_k^\dagger a_l^\dagger a_n a_m \tag{12.25}$$

this is a microscopic description of valence particles around Fermi energy (HF maybe). Here

e_k are the single particles energies in deformed Nilsson potential (for example). The collective part reads

$$H_{coll} = \sum_{i=1}^{3} \frac{R_i^2}{2\mathcal{I}_i} \tag{12.26}$$

R_i are the body-fixed collective angular momenta of the core. Given the angular momentum of the valence particle $\boldsymbol{j}$ they form $\boldsymbol{I} = \boldsymbol{R} + \boldsymbol{j}$ is the total angular momentum. Eliminating R we can rewrite the Hamiltonian as

$$H_{coll} = \sum_{i} \frac{I_i^2}{2\mathcal{I}_i} + \frac{j_i^2}{2\mathcal{I}_i} - \frac{I_i j_i}{\mathcal{I}_i} \tag{12.27}$$

The first term acts only on the degrees of freedom of the rotor; the second on the coordinates of the valence particle and the last term is the 'Coriolis' term.

Let's assume axial symmetry so that $\mathcal{I}_1 = \mathcal{I}_2 = \mathcal{I}$. No rotation in q.m. along the symmetry axis (3-axis). It follows that the 3-component of of the total angular momentum I has to be equal to the 3-component of j

$$K = \Omega \tag{12.28}$$

We thus obtain

$$H_{coll} = \frac{\boldsymbol{I}^2 - I_3^2}{2\mathcal{I}} + \frac{j_1^2 + j_2^2}{2\mathcal{I}} - \frac{1}{\mathcal{I}}(I_1 j_1 + I_2 j_2) \tag{12.29}$$

The recoil term acts only in the intrinsic coordinates. We can neglect if we adjust the intrinsic degrees of freedom to experiment!

To solve such a system we can consider 3 limiting cases:

1. strong coupling limit: the odd particle adiabatically follows the rotation of the even core. It is realised if the coupling to the deformation is much stronger than the perturbation induced by Coriolis.

2. weak coupling limit: very small deformations, the odd particle moves on spherical shell model levels only slightly disturbed by other effects (quadrupole vibrations for example)

3. decoupling limit: the Coriolis is so strong that the coupling to the deformation of the core can be neglected

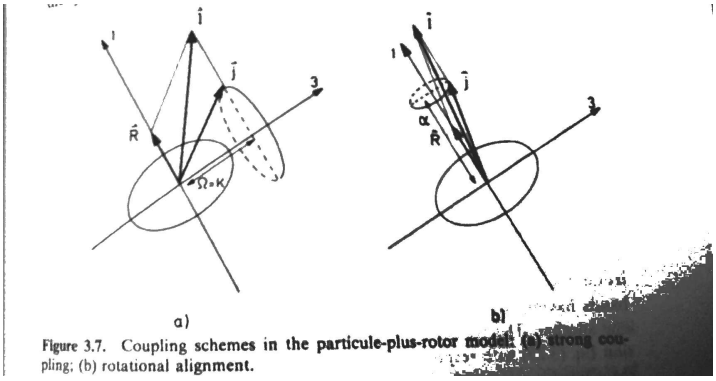

Figure 3.7. Coupling schemes in the particule-plus-rotor model: (a) strong coupling; (b) rotational alignment.

Figure 12.4: Schematic representation of the particle-rotor coupling. Taken from [45]

12.2.1 Strong coupling

The strong limit is realized when the Coriolis term is small compared to the level splitting of single particle energies. This is the case

- large deformations, because of the splitting in Nilsson Hamiltonian is proportional to deformation.
- Coriolis is small. Small values of j or low spins I.

This limit is called strong coupling or deformation aligned because in the case K is a good quantum number. The angular momentum j os the valence particle is strongly coupled to the motion of the core. In a semiclassic picture j precesses around the 3-axis (left panel of Fig.12.4) Since Coriolis is the only term that couples the rotor degrees of freedom with the intrinsic one, we can factorise the w.f. in terms of inner degrees of freedom ϕ^i_K and rotor w.f. $|IMK\rangle$

We assume that (adiabatic approximation) that the rotational motion has no influence on the inner structure. The projection of the total angular momentum K along the symmetry axis is a good quantum number. The term $j_1^2 + j_2^2$ depend only on single particle w.f. ϕ_ν and they are thus constant along the rotational band. We ignore them also at first order.

The total energy reads

$$E_{IK} = |e_\nu - \lambda| + \frac{\hbar^2}{2\mathcal{I}}\left[I(I+1) - K^2\right] \tag{12.30}$$

Usually we should have quasi-particle $\rightarrow$ pairing. The lowest possible spin is $I_0 = K$. The band-head $E(I_0)$ is not precisely e_K but slightly shifted especially if we take into account the terms we have neglected. The spectrum has a spacing of $\Delta I = 1$ and its moment of inertia is that of the rotor

$$\mathcal{I} \approx \frac{\beta^2 A^{7/3}}{400} \text{ MeV}^{-1} \tag{12.31}$$

The energy of the band should be corrected by the Coriolis term $I \cdot j$.

If we take into account Coriolis we get a contribution in first order perturbation theory only for $K = 1/2$ as

$$E_{Coriolis} = \frac{\hbar^2}{2\mathcal{I}} a^i \left(I + \frac{1}{2} \right) (-)^{I+1/2} \tag{12.32}$$

where a^i is the *decoupling* factor. This introduces a small distortion to the rotational spectrum. This term is used to explain the distortion observed in K=1/2 band. The Coriolis term can also explain the coupling between K=1/2 and K=-1/2 bands.

12.2.2 Weak coupling

As said before the strong coupling breaks down if Coriolis is not negligible compared to single particle energies belonging to different K values. (ψ^I_{MK} is the total w.f. of the system)

$$\langle \psi^I_{MK+1} | H_{Cor} | \psi^I_{MK} \rangle = -\frac{1}{\mathcal{I}} \sqrt{I(I+1) - K(K+1)} \langle \psi_{\Omega+1} | j_x | \psi_\Omega \rangle \tag{12.33}$$

if $|\psi^i_\Omega\rangle = \sum_{nj} C^i |nj\Omega\rangle$ is decomposed on eigenstates of j^2; we can calculate the matrix element as

$$\langle \psi^I_{MK+1} | H_{Cor} | \psi^I_{MK} \rangle = -\frac{1}{\mathcal{I}} \sum_{nj} |C_n j|^2 \sqrt{I(I+1) - K(K+1)} \sqrt{j(j+1) - \Omega(\Omega+1)} \tag{12.34}$$

so the matrix elements are large for large values of I/K and j/Ω. That is for example the case of levels with large values of j and small Ω are involved.

In the current weak limit, we neglect the K-splitting of the intrinsic degrees of freedom (small deformation). In this case $[j^2, R^2]$[1] commute with H_{int}. The corresponding spectrum will look like

$$E(I) = E_{int} + \frac{1}{2\mathcal{I}} R(R+1) \tag{12.35}$$

with $|j - R| \leq I \leq j + R$. and $R = 0, 2, 4, ...$ Why only even number? Because it turns out that the Hamiltonian of a rotor has an extra symmetry $\mathcal{R} = e^{i\pi \hat{I}_1}$. See Bohr-Mottelson book

[1] Remember that $\boldsymbol{R} = \boldsymbol{I} - \boldsymbol{j}$

for details. This symmetry is equivalent to a reflection with respect to the plane 2,3-plane together with a parity transformation.

This means that for each rotational quantum number R, j can have 2j+1 orientations without changing the energy of the system. The splitting of these levels can be taken into account by first order perturbation theory. $\beta\hbar\omega_0\langle\psi_M^{IR}|r^2Y_{20}|\psi_M^{IR}\rangle$.

$$E(I) = E_{int} + \frac{1}{2\mathcal{I}}R(R+1) - \beta\hbar\omega_0\langle\psi_M^{IR}|r^2Y_{20}|\psi_M^{IR}\rangle \tag{12.36}$$

For each orientation of $\boldsymbol{j}$ there is a whole rotational band of the core with $\Delta R = 2$. The levels with the highest values of I=R+j for a given energy correspond to the yras levels. These levels are connected by strong E2 transitions They are called *favoured states* and their energy is given by

$$E(I) = E_{int} + \frac{1}{2\mathcal{I}}(I-j)(I-j+1) \tag{12.37}$$

The states lie on a parabola with minimum $I \approx j$.

12.2.3 Decoupling limit

In this case we can not neglect the splitting of levels in the intrinsic part. We write the Hamiltonian as

$$H = H_{sp} + \frac{\hbar^2}{2\mathcal{I}}(I^2 + j^2 - 2I\cdot j) \tag{12.38}$$

We want to minimise the total energy so for given I and more or less fixed j. The $I\cdot j$ of the rotor tries to align the intrinsic spin j with the total spin I. The latter is in most cases perpendicular to the symmetry axis (3-axis) There will be a tendency toward a large perpendicular component of j contrary to the aligned case where j is quantised along the symmetry axis. See right panel of Fig.12.4 We get

$$E = \frac{\hbar^2}{2\mathcal{I}}\left[I(I+1) + j(j+1) - 2\Omega K + a(-)^{I+1/2}\left(I+\frac{1}{2}\right)\right] \tag{12.39}$$

where we consider for example j=13/2 and $\Omega = K = 1/2$. Why $i_{13/2}$, since this is intruder state and it is 'uncoupled' to surrounding orbitals of different parity.

We thus observe that if we take the band with $I = j, j+2, j+4, ...$ in the aligned case. the spin projection on the rotation axis equal j and the total rotational energy can be written as

$$
\begin{aligned}
E &= \frac{\hbar^2}{2\mathcal{I}}\left[I(I+1)+j(j+1)-2I\alpha\right] && (12.40)\\
&= \frac{\hbar^2}{2\mathcal{I}}\left[(I-\alpha)(I-\alpha+1)-2\alpha\right] && (12.41)\\
&= \frac{\hbar^2}{2\mathcal{I}}\left[R(R+1)\right]+const && (12.42)
\end{aligned}
$$

with $R = I - \alpha$ describes the collective motion.

12.3 Exercise

Prove the relation

$$
\langle Nlsj\Omega|\varepsilon h'|Nlsj\Omega\rangle = \frac{1}{6}\varepsilon M\omega_0^2\langle r^2\rangle\frac{3\Omega^2-j(j+1)}{j(j+1)} \tag{12.43}
$$

where

$$
\begin{aligned}
\varepsilon h' &= \varepsilon\frac{M}{2}\frac{2}{3}\omega_0^2(x^2+y^2-2z^2) = -M\omega_0^2\frac{2}{3}\varepsilon r^2 P_2(\cos\theta) && (12.44)\\
\phi(Nlsj\Omega)(r,\theta) &= R_{Nl}(r)\sum_{\Lambda\Sigma} C^{j\Omega}_{l\Lambda\frac{1}{2}\Sigma}Y_{l\Lambda}(\theta)\chi_{\frac{1}{2}\Sigma} && (12.45)\\
\langle r^2\rangle &= \int dr r^4 R_{Nl}^2(r) && (12.46)
\end{aligned}
$$

Lecture 13

Computational DFT [Week 3 day 3]

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13.1 General Considerations on HFB Solvers

13.1.1 Strategies for Solving the HFB Equation

Reminder

$$[\mathcal{H}, \mathcal{R}] = 0 \tag{13.1}$$

Two main methods to solve the HFB equation

- Non-linear eigenvalue problem in configuration space (=basis)

- Initialize density $\mathcal{R} \equiv \mathcal{R}^{(0)}$ (that is, $\rho^{(0)}$ and $\kappa^{(0)}$);
- Use these densities to compute the HFB matrix at 0-iteration $\mathcal{H}^{(0)}$;
- Diagonalize $\mathcal{H}^{(0)}$ to obtain eigenvectors $\begin{pmatrix} U^{(0)} \\ V^{(0)} \end{pmatrix}$
- Calculate new densities

$$\rho^{(1)} = V^{(0)*}V^{(0)T}, \quad \kappa^{(1)} = V^{(0)*}U^{(0)T}$$

- Use the new densities to recalculate HFB matrix at 1-iteration $\mathcal{H}^{(1)}$
- Repeat until densities (or other relevant quantities) do not change.

- Gradient method based on the Thouless theorem in configuration space
  - Initialize Bogoliubov transformation $\mathcal{W}^{(0)}$ (hence the $U^{(0)}$ and $V^{(0)}$)
  - Calculate generalized density $\mathcal{R}^{(0)}$ from $W^{(0)}$ and from there the HFB matrix at 0-iteration $\mathcal{H}^{(0)}$
  - Compute $\mathcal{Z} = i\eta[\mathcal{R}^{(0)}, \mathcal{H}^{(0)}]$ with $\eta \ll 1$ (until convergence, the commutator is not zero)
  - Construct new iteration of Bogoliubov matrix by

$$\mathcal{R}^{(1)} = \mathcal{R}^{(0)} + i[\mathcal{Z}, \mathcal{R}^{(0)}]$$

    and recalculate the HFB matrix at 1-iteration $\mathcal{H}^{(1)}$
  - Repeat until nothing changes

Note: for the HF+BCS equation, the imaginary time method can also be used.

- Basis expansion of HFB wave functions

$$\begin{pmatrix} h-\lambda & \Delta \\ -\Delta^* & -h^*+\lambda \end{pmatrix} \begin{pmatrix} U_\mu \\ V_\mu \end{pmatrix} = E_\mu \begin{pmatrix} U_\mu \\ V_\mu \end{pmatrix} \tag{13.2}$$

with

$$\begin{pmatrix} U_\mu(\boldsymbol{r}\sigma) \\ V_\mu(\boldsymbol{r}\sigma) \end{pmatrix} \equiv \sum_{n=1}^{N_{\text{basis}}} \begin{pmatrix} U_{n\mu} \\ V_{n\mu} \end{pmatrix} \varphi_n(\boldsymbol{r}\sigma) \tag{13.3}$$

- Direct r-space discretization of HFB equation

$$\int d^3\boldsymbol{r}' \sum_{\sigma'} \begin{pmatrix} h(\boldsymbol{r}\sigma,\boldsymbol{r}\sigma') - \lambda\delta_{\sigma\sigma'} & \Delta(\boldsymbol{r}\sigma,\boldsymbol{r}\sigma')\delta_{\sigma\sigma'} \\ -\Delta(\boldsymbol{r}\sigma,\boldsymbol{r}\sigma')\delta_{\sigma\sigma'} & -h(\boldsymbol{r}\sigma,\boldsymbol{r}\sigma') + \lambda\delta_{\sigma\sigma'} \end{pmatrix} \begin{pmatrix} U_\mu(\boldsymbol{r}\sigma) \\ V_\mu(\boldsymbol{r}\sigma) \end{pmatrix} = E_\mu \begin{pmatrix} U_\mu(\boldsymbol{r}\sigma) \\ V_\mu(\boldsymbol{r}\sigma) \end{pmatrix} \tag{13.4}$$

with

$$\begin{pmatrix} U_\mu(\boldsymbol{r}\sigma) \\ V_\mu(\boldsymbol{r}\sigma) \end{pmatrix} \equiv \begin{pmatrix} U_\mu(\boldsymbol{r}_i\sigma) \\ V_\mu(\boldsymbol{r}_i\sigma) \end{pmatrix}, \quad i = 1, \ldots, N_{\text{points}} \tag{13.5}$$

- Lattice representation of coordinate space (Lagrange meshes, spline meshes, etc.)

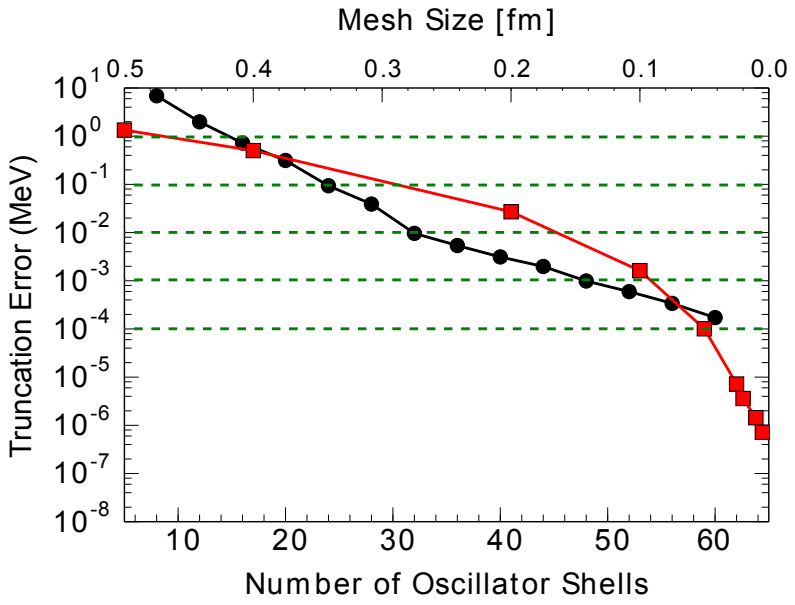

Figure 13.1: **Convergence of a HFB calculation for ^{208}Pb, both as a function of the number of shells in the HO basis (black circles, lower x-axis) and as a function of the mesh size in coordinate space (red squares, upper x-axis).**

13.1.2 Types of Energy Functionals

Popular EDF in nuclear physics: Skyrme and Gogny

- Skyrme potential is local, zero-range

$$\hat{V}_{\text{Skyrme}}(\boldsymbol{r}_1, \boldsymbol{r}_2) \propto \delta(\boldsymbol{r}_1 - \boldsymbol{r}_2)\delta(\boldsymbol{r}_1 - \boldsymbol{r}_1')\delta(\boldsymbol{r}_2 - \boldsymbol{r}_2') \tag{13.6}$$

  which leads to a functional of the local density $\rho(\boldsymbol{r})$ and derivatives $\tau(\boldsymbol{r})$, etc.,

$$E[\rho] = \int d^3\boldsymbol{r}\ \mathcal{H}(\boldsymbol{r}), \qquad \mathcal{H}(\boldsymbol{r}) = C^{\rho\rho}\rho^2 + C^{\rho\tau}\rho\tau + \ldots \tag{13.7}$$

- Gogny potential is local, finite range

$$\hat{V}_{\text{Gogny}}(\boldsymbol{r}_1, \boldsymbol{r}_2) \propto e^{-(\boldsymbol{r}_1 - \boldsymbol{r}_2)^2/\mu^2}\delta(\boldsymbol{r}_1 - \boldsymbol{r}_1')\delta(\boldsymbol{r}_2 - \boldsymbol{r}_2') \tag{13.8}$$

  which leads to a functional of the non-local density $\rho(\boldsymbol{r}, \boldsymbol{r}')$,

$$E[\rho] = \int d^3\boldsymbol{r} \int d^3\boldsymbol{r}'\ \mathcal{H}(\boldsymbol{r}, \boldsymbol{r}'), \qquad \mathcal{H}(\boldsymbol{r}, \boldsymbol{r}') = C^{\rho\rho}\rho^2(\boldsymbol{r}, \boldsymbol{r}')e^{-(\boldsymbol{r} - \boldsymbol{r}')^2/\mu^2} + \ldots \tag{13.9}$$

Next generation of EDF

- Three- and Four-body potentials $V(\boldsymbol{r}_1, \boldsymbol{r}_2, \boldsymbol{r}_3)$, $V(\boldsymbol{r}_1, \boldsymbol{r}_2, \boldsymbol{r}_3, , \boldsymbol{r}_4)$
- Momentum-dependent potential

Possible computational bottlenecks

- In configuration space, one needs to compute *tensor contractions* of the type

$$\sum_{abcd} \bar{v}_{abcd}\rho_{db} \text{ (NN)} \quad \text{or} \quad \sum_{abcdef} \bar{v}_{abcdef}\rho_{eb}\rho_{fc} \text{ (NNN)}$$

  with $a \equiv (n, \ell, j, m)$ or $a \equiv (n_x, n_y, n_z, \sigma), \ldots$

- In coordinate space, one must perform multi-dimensional integrals and differentiation such as

$$\int d^3\boldsymbol{r} \int d^3\boldsymbol{r}' V(\boldsymbol{r}-\boldsymbol{r}')\rho(\boldsymbol{r},\boldsymbol{r}')\rho(\boldsymbol{r}',\boldsymbol{r}) \quad \text{and} \quad \boldsymbol{\nabla}\cdot\boldsymbol{\nabla}\rho(\boldsymbol{r}',\boldsymbol{r})$$

13.1.3 Symmetries (and lack thereof)

13-1: Conserved symmetries and block structure

> For any self-consistent symmetry $\mathcal{S}$, the density matrix and pairing tensor, and the Hartree-Fock potential and pairing field, can be put into a block diagonal form in the basis of the eigenstates of the symmetry operators.

Usual example: if rotational invariance is a self-consistent symmetry, then

$$[\hat{h}, \hat{j}^2] = [\hat{h}, \hat{l}^2] = 0 \tag{13.10}$$

Define a basis of states $\varphi_{n\ell jm}(\boldsymbol{r})$ that are eigenstates of $\hat{j}^2$ and $\hat{\ell}^2$. In that basis,

$$h_{\alpha\beta} = \begin{pmatrix} \ddots & & & & 0 \\ & \begin{bmatrix} \ddots & & \\ & h^{(\ell j)}_{\alpha\beta} & \\ & & \ddots \end{bmatrix} & & & \\ & & & & \\ 0 & & & & \ddots \end{pmatrix} \tag{13.11}$$

Therefore, diagonalization of the HF (and HFB) matrix can be performed by block, which is advantageous since the time of diagonalization scales like $\mathcal{O}(N^3)$ with N the size of the matrix.

Estimates of runtime for full HFB solution on current architectures

Additional advantage: each s.p. or q.p. states gets a label corresponding to the conserved quantum numbers associated with the symmetry.

1D (spherical)	2D (axial)	3D (triaxial)
< 10 s	< 10 min	< 10 hours

Table 13.1: **Time to solution for HFB equation in a large HO basis ($N_0 = 20$) for the ground-state of an even-even nucleus with a Skyrme force.**

13.1.4 Configuration Space

Choice of basis functions sometimes matter

- Physical wavefunctions of the nucleus should fall like e^{-kr} for large r but eigenfunctions of the HO behave like Gaussians (no matter which coordinate system) and do not have the proper asymptotic behavior

- On the other hand, eigenfunctions of a finite potential (square well, Woods-Saxon, Nilsson) are mostly non-localized (=continuum states) and may not be adapted to describing a well-bound nucleus with good precision

- Basis functions centered at the origin (HO, WS, square well, etc.) are not well adapted at describing very deformed shapes (fission, reaction)

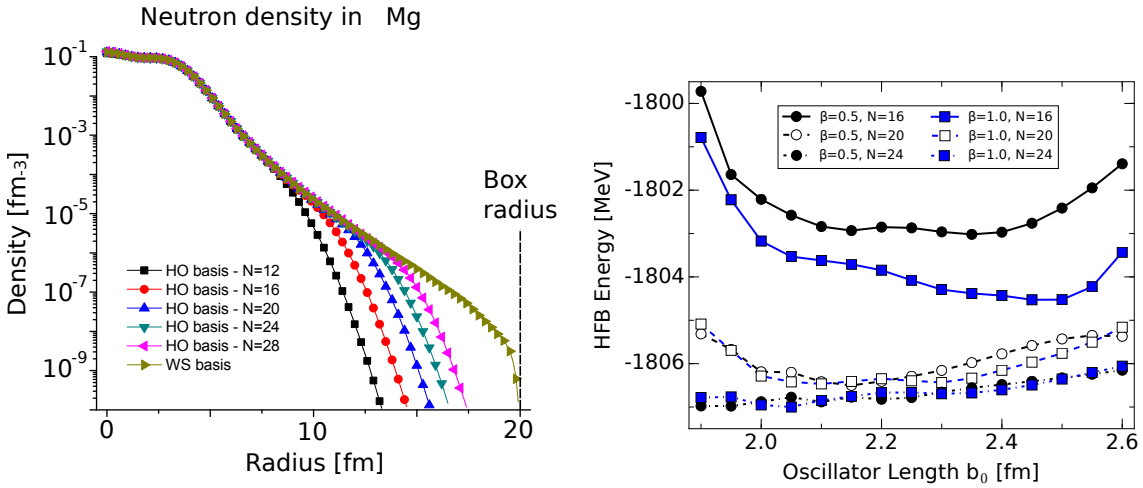

Figure 13.2: **Left: Radial density in ^{40}Mg as a function of r computed by expanding the HFB solution either on the HO basis or on the WS basis. Right: convergence of the HFB energy as a function of the HO basis characteristics for a very deformed configuration in ^{240}Pu ($\langle \hat{Q}_{20} \rangle = 200$ b, $\langle \hat{Q}_{20} \rangle = 50$ b^2)**

Asymptotic behavior of wavefunctions especially relevant for reaction theory, not so much for structure.

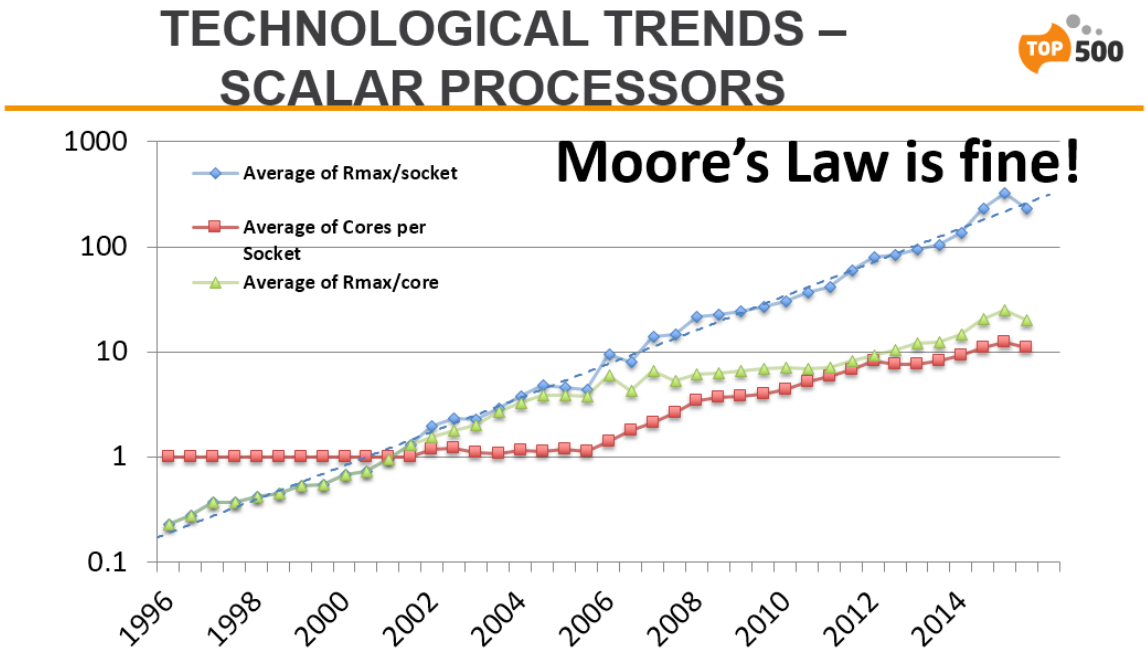

Figure 13.3: **Evolution of Flops/socket as a function of time. The traditional Moore's law has been broken already 10 years ago...**

13.2 Algorithms, Optimization and Parallelism

13.2.1 Reminder on Parallel Computing

CPU speed has not improved significantly over the past decade: gains in computational power have come almost exclusively from an increase in parallelism.

Two different types of parallelism (to simplify)

- Shared memory parallelism (OpenMP, Pthreads) – Different CPU (typically between 4 and 24) share the same block of physical memory.
  - Advantages: usually implemented via pragmas – commented lines in the source code that are interpreted only if the code is compiled in a certain way.
  - Drawbacks: scalability is very limited. API not always consistent
- Distributed memory parallelism (MPI) – CPU are located on different chips that do not have access to the same memory. Explicit communication to exchange data is needed.
  - Advantages: scalable and programmer is in control of what (s)he is doing
  - Drawbacks: requires an implementation (=library) and adding in the source file all instructions needed to do the communication

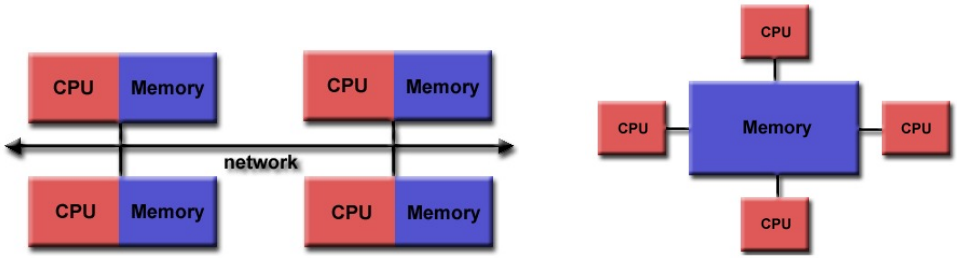

Figure 13.4: **Left: Distributed memory parallelism. Right: shared memory parallelism.**

13.2.2 OpenMP

```
Program test_OpenMP
  Implicit none
  Integer :: i,N
  Integer, allocatable :: A(:)

  N = 10000000
  Allocate(A(1:N))
  Write(*,'("Hello World in serial region")')

!$OMP PARALLEL SHARED(A,N) PRIVATE(I)
!$OMP DO
  Do i=1,N
     A(i) = i
  End Do
!$OMP END DO
!$OMP END PARALLEL

  Open(55,file='toto.dat',form='formatted')
  Write(55,*) A
  Close(55)

End Program test_OpenMP
```

How it works:

- OpenMP capabilities are inserted in the form of *comments* that are only interpreted when the code is compiled with specific flags
- Until the `!$OMP PARALLEL`, the code is executed serially as usual
- Between `!$OMP PARALLEL` and `!$OMP END PARALLEL`, the code creates several *threads* (controlled by the environment variable `OMP_NUM_THREADS`) that have all access to the same variables. In our example, work to set $A_i = i$ for a vector of size N is divided between available threads. Both the vector and its size are shared by all threads (*public variables*), while the running index is specific to each thread (*private variable*).

13.2.3 MPI

```
Program test_MPI
  Include 'mpif.h'
  Integer :: mpi_err, mpi_size, mpi_rank

  Call mpi_init(mpi_err)
  Call mpi_comm_size(MPI_COMM_WORLD, mpi_size, mpi_err)
  Call mpi_comm_rank(MPI_COMM_WORLD, mpi_rank, mpi_err)

  If (mpi_rank.Eq.0) Then
     Write(6,'("The master says Hello")')
  Else
     Write(6,'("The slave",i4," is sulking")') mpi_rank
  End if

  Call mpi_finalize(mpi_err)

End Program test_MPI
```

How it works:

- The code must be compiled with calls to proper libraries. Typically, MPI installation provides a wrapper such as `mpif90` or `mpif77` which can be used instead of your favorite compiler.
- Run the code by specifying the number of MPI tasks with something like

  ```
  mpirun -np 4 test_MPI
  ```

- At execution, everything happens *as if the executable were cloned in* `np` *copies*
  - Each clone is independent of the others to start with
  - Use calls to basic MPI routines to access process number in source code and enable communication among processes
  - Beware of naive statements such as `write(6,*)`: all processes will try to write to the *same* standard output...
- When coding, always imagine what the code would/should do if it is run by the process number [something]
- More advanced routines allow the partitioning of all available processes into specific groups (=communicators). A given process may belong to different communicators.

13.2.4 Optimization

Loop nesting - Memory storage of arrays depends on programming language: accessing large multidimensional arrays in nested loops must be coded differently in Fortran and C

Fortran

```
sum_A = 0.0
do k=1,N
   do j=1,N
      do i=1,N
         sum_A = sum_A + A(i,j,k)
      end do
   end do
end do
```

C

```
sum_A = 0.0;
for (i=1; i<=N; i++)
    {
    for (j=1; j<=N; j++)
        {
        for (k=1; k<=N; k++)
            { sum_A = sum_A + A[i,j,k]; }
        }
    }
```

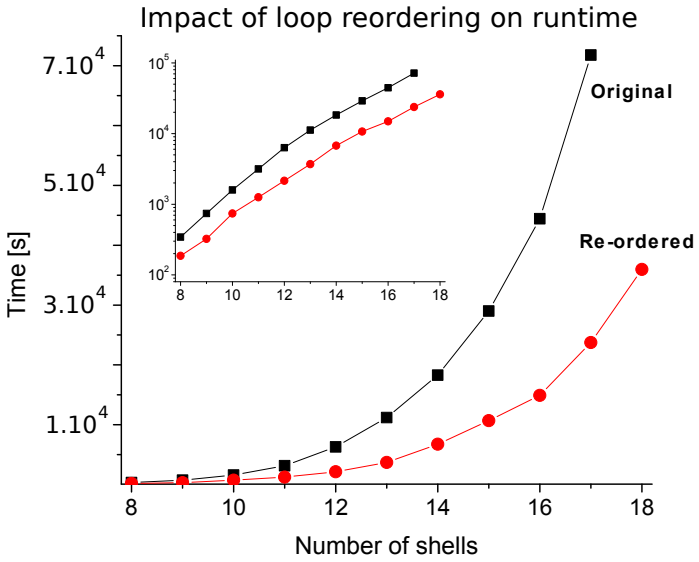

Figure 13.5: **Impact of loop reordering on the calculation of the mean-field Γ_{nm} for a Gogny potential.**

Memory and algorithms - The number of matrix elements $\langle ab|\hat{v}|cd\rangle$ for a two-body interaction in a basis with $N_0 = 20$ shells depends dramatically on the conserved symmetries

	1D (spherical)	2D (axial)	3D (triaxial)
scaling	$\approx N_0^5$	$\approx N_0^9$	$\approx N_0^{12}$
size	≈ 1 MB	≈ 1 GB	≈ 1 TB

Table 13.2: **Characteristics of matrix elements needed to solve the HFB equations for different symmetries**

Consequence: for 2D and 3D geometries, it is not efficient to precalculate the matrix elements and access them when computing Γ_{ij} and/or Δ_{ij}.

- Alternative 1: calculate fields on-the-fly (CPU-dependent)
- Alternative 2: use large-scale parallelism (communication-dependent)

Algorithms - Consider the mean-field potential for a generic (but separable) two-body force in Cartesian coordinates

$$\Gamma_{ij} \equiv \Gamma_{\boldsymbol{nm}}, \quad \boldsymbol{n} = n_x, n_y, n_z \tag{13.12}$$

A naive calculation could involve the (utterly horrible) code below

```
do nx=1,N
   do ny=1,N
      do nz=1,N
         do mx=1,N
            do my=1,N
               do mz=1,N
                  do npx=1,N
                     do npy=1,N
                        do npz=1,N
                           do mpx=1,N
                              do mpy=1,N
                                 do mpz=1,N
  gamma(nx,ny,nz,mx,my,mz) = gamma(nx,ny,nz,mx,my,mz) &
+ twobody(nx,ny,nz,npx,npy,npz,mx,my,mz,mpx,mpy,mpz)  &
* rho(mpx,mpy,mpz,npx,npy,npz)
                                 end do
                              end do
                           end do
                        end do
                     end do
                  end do
               end do
            end do
         end do
      end do
   end do
end do
```

What is wrong here:

- 12-nested loop will be *extremely* slow
- 12-dimensional arrays will require *prohibitive* storage, see table 13.2
- no advantage taken of separability of interaction
- no advantage taken of parallelism

Use the fact that the potential is separable. Example: the Gogny force

$$V(\boldsymbol{r}, \boldsymbol{r}') = e^{-\frac{(\boldsymbol{r}-\boldsymbol{r}')^2}{\mu^2}} = e^{-\frac{(x-x')^2}{\mu^2}} e^{-\frac{(y-y')^2}{\mu^2}} e^{-\frac{(z-z')^2}{\mu^2}} \tag{13.13}$$

therefore

$$\Gamma_{\boldsymbol{n'm'}} = \sum_{n'_x m'_x} V_{n_x n'_x m_x m'_x} \sum_{n'_y m'_y} V_{n_y n'_y m_y m'_y} \sum_{n'_z m'_z} V_{n_z n'_z m_z m'_z} \rho_{\boldsymbol{mn}} \tag{13.14}$$

Separate contributions from each direction as follows (red indices imply summations, but not contractions)

$$Y^{n'_z m'_z}_{m_x n_x m_y n_y} = \sum_{n'_z m'_z} \sum_{n_z m_z} V_{n_z n'_z m_z m'_z} \rho_{m_x m_y m_z n_x n_y n_z} \tag{13.15}$$

$$Z^{n'_z m'_z n'_y m'_y}_{m_x n_x} = \sum_{n'_y m'_y} \sum_{n_y m_y} V_{n_y n'_y m_y m'_y} Y^{n'_z m'_z}_{m_x n_x m_y n_y} \tag{13.16}$$

$$\Gamma^{n'_z m'_z n'_y m'_y n'_x m'_x} = \sum_{n'_x m'_x} \sum_{n_x m_x} V_{n_x n'_x m_x m'_x} Z^{n'_z m'_z n'_y m'_y}_{m_x n_x} \tag{13.17}$$

```
G(:,:) = 0.0
do nx=1,N
   do mx=1,N

      do ny=1,N
         do my=1,N

            do npz=1,N
               do mpz=1,N

                  D=0.0
                  do nz=1,N
                     do mz=1,N
                        i = indexv(mx,my,mz)
                        j = indexv(nx,ny,nz)
                        D = D + V(mz,nz,mpz,npz) * rho(j,i)
                     end do
                  end do
                  Y(my,ny,mpz,npz)=D

               end do
            end do

         end do
      end do

      do npz=1,N
         do mpz=1,N

            do npy=1,N
               do mpy=1,N

                  D=0.0
                  do ny=1,N
                     do my=1,N
                        D = D + V(my,ny,mpy,npy) * Y(my,ny,mpz,npz)
                     end do
```

```
                    end do
                    Z(mpy,npy,mpz,npz)=D

                end do
            end do
        end do

        do npz=1,N
            do mpz=1,N

                do npy=1,N
                    do mpy=1,N

                        do npx=1,N
                            do mpx=1,N
                                i = indexv(mpx,mpy,mpz)
                                j = indexv(npx,npy,npz)
                                G(i,j) = G(i,j) + V(mx,nx,mpx,npx) &
                                                *Z(mpy,npy,mpz,npz)
                            end do
                        end do

                    end do
                end do
            end do
        end do

    end do
end do
```

Scales like $\mathcal{O}(N^8)$

Parallelism - Continue on the example above, but take advantage of the fact that several loops can be parallelized.

```
G(:,:) = 0.0

! rank of the current CPU in the group dedicated to the mean-field
! calculation
Call mpi_comm_rank(group_comm, group_rank, mpi_err)
! Size of said group
Call mpi_comm_size(group_comm, group_size, mpi_err)

do nx=1,N
    ! Conditional execution: only for those values of Nx that match
    ! this pattern do we do the calculation
    If (group_rank .Eq. Mod(Nx,group_size)) Then
        do mx=1,N
```

```
        ⋮
end do

! Size of the matrix G
buffer_size = Nmax*Nmax

! New matrix containing the full matrix G
Allocate(full_G(Nmax,Nmax)

! Combine matrices of each rank into a single one
Call mpi_allreduce(G, full_G, buffer_size, MPI_DOUBLE_PRECISION, &
                   MPI_SUM, group_comm, mpi_err)
```

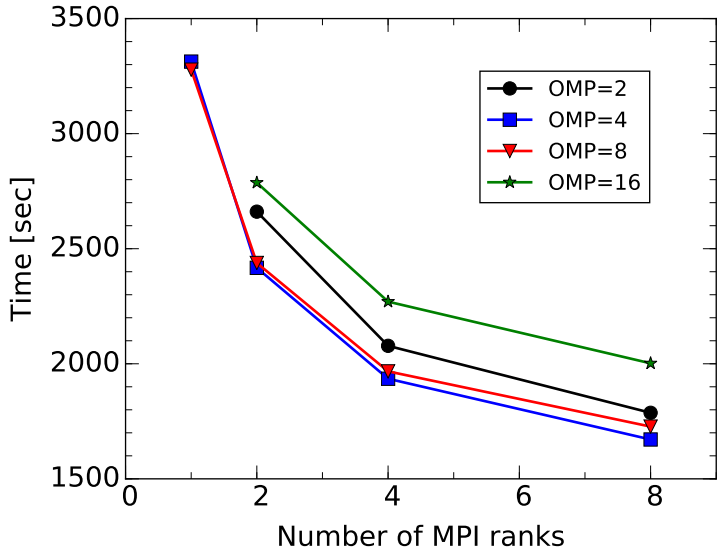

Figure 13.6: **Acceleration of triaxial Gogny calculations in a large HO basis as a function of MPI tasks and OpenMP threads.**

13.3 Beyond HFB

13.3.1 RPA and QRPA

Recall that the RPA equations for channel ν are

$$\begin{pmatrix} A & B \\ -B^* & -A^* \end{pmatrix} \begin{pmatrix} X_\nu \\ Y_\nu \end{pmatrix} = \Omega_\nu \begin{pmatrix} X_\nu \\ Y_\nu \end{pmatrix} \tag{13.18}$$

with

$$\begin{aligned} A_{ph,p'h'} &= (\varepsilon_p - \varepsilon_h)\delta_{pp'}\delta_{hh'} + \bar{v}_{ph'hp'} \\ B_{ph,p'h'} &= \bar{v}_{pp'hh'}. \end{aligned} \tag{13.19}$$

Diagonalizing the RPA matrix in the general case

- h runs over all occupied HF states – possibly including both neutrons and protons states, say $h = 1, \ldots, 100$
- p runs over a set of "relevant" empty states. For sake of simplicity, assume again $p = 1, \ldots, 100$
- Total number of ph states is $100 \times 100 = 10^4$: diagonalize dense (=lots of non-zero matrix elements) matrices of size $10^4 \times 10^4$.

Still doable, but RPA misses important correlations for open shell nuclei

QRPA equations for channel ν take a very similar form as RPA

$$\begin{pmatrix} A & B \\ -B^* & -A^* \end{pmatrix} \begin{pmatrix} X_\nu \\ Y_\nu \end{pmatrix} = \Omega_\nu \begin{pmatrix} X_\nu \\ Y_\nu \end{pmatrix} \tag{13.20}$$

with, this time (Einstein's summation conventions apply)

$$\begin{aligned} A_{ij\mu\nu} = & \ (E_i + E_j)\delta_{i\mu}\delta_{j\nu} \\ & + \ U^\dagger_{i\alpha} V^*_{\beta j} \bar{v}_{\alpha k \beta l} U_{l\mu} V^T_{\nu k} - V^\dagger_{i\alpha} V^*_{\beta j} \bar{v}^*_{\alpha\beta kl} V_{k\nu} V^T_{\mu l} \\ & + \ U^\dagger_{i\alpha} U^*_{\beta j} \bar{v}_{\alpha\beta kl} U_{k\mu} U^T_{\nu l} - V^\dagger_{i\alpha} U^*_{\beta j} \bar{v}^*_{\alpha k \beta l} V_{l\nu} U^T_{\mu k} \\ B_{ij\mu\nu} = & \ -U^\dagger_{i\alpha} V^*_{\beta j} \bar{v}_{\alpha k \beta l} V^*_{l\nu} U^\dagger_{\mu k} + V^\dagger_{i\alpha} V^*_{\beta j} \bar{v}^*_{\alpha\beta kl} U^*_{k\mu} U^\dagger_{\nu l} \\ & -U^\dagger_{i\alpha} U^*_{\beta j} \bar{v}_{\alpha\beta kl} V^*_{k\nu} V^\dagger_{\mu l} + V^\dagger_{i\alpha} U^*_{\beta j} \bar{v}^*_{\alpha k \beta l} U^*_{l\mu} V^\dagger_{\nu k} \end{aligned} \tag{13.21}$$

New estimates of the size in the general case

- every index i, j, μ, ν runs over the size of the s.p. basis – unless the number of quasiparticles (=eigenvectors) is truncated. Suppose a basis of $N = 1,000$ states.
- Total number of ij or $\mu\nu$ states is now $1,000 \times 1,000 = 10^6$: diagonalize dense matrices of size $10^6 \times 10^6$.

Simplifications: use self-consistent symmetries (but lose some physics).

13.3.2 GCM and Projection

Particle number projection - Project on both protons and neutrons

$$E_{\rm PAV} = \frac{1}{2\pi} \int d\varphi_n \int d\varphi_p \; y(\varphi_n, \varphi_p) E(\varphi_n, \varphi_p) \tag{13.22}$$

with

$$E(\varphi_n, \varphi_p) = \sum_{\tau\tau'} E^{\tau\tau'}(\varphi_\tau, \varphi_{\tau'}), \qquad \tau, \tau' = n, p \tag{13.23}$$

and

$$\begin{aligned} E^{\tau\tau}(\varphi,\varphi) &= t_{ij}\rho^{\tau}_{ji}(\varphi) + \frac{1}{2}\Gamma^{\tau\tau}_{ij}(\varphi)\rho^{\tau}_{ji}(\varphi) - \frac{1}{2}\Delta^{\tau\tau}_{ij}(\varphi)\kappa^{\tau}_{ji}(\varphi) \\ E^{\tau\tau'}(\varphi,\varphi') &= \frac{1}{2}\Gamma^{\tau\tau'}_{ij}(\varphi')\rho^{\tau}_{ji}(\varphi) \end{aligned} \tag{13.24}$$

Bottom line: when discretizing the integrals over gauge angle with N quadrature points, you need to recalculate N^2 HFB-like energies. Typically, $N = 7$ is sufficient.

Angular momentum projection - Take a triaxial deformed HFB state $|\Phi\rangle$ and project on good angular momentum

$$|IMK\rangle = \frac{2I+1}{8\pi^2}\int d\Omega \mathcal{D}^{I*}_{ML}(\Omega)\hat{R}(\Omega)|\Phi\rangle \tag{13.25}$$

with $\Omega = (\alpha, \beta, \gamma)$ the Euler angles, $\mathcal{D}^{I*}_{ML}(\Omega)$ Wigner matrices and $\hat{R}(\Omega)$ a rotation operator defined as

$$\hat{R}(\Omega) = e^{-i\alpha\hat{I}_x}e^{-i\beta\hat{I}_y}e^{-i\gamma\hat{I}_z}$$

For $I = 10$, you need at least 20 points for each Euler angle (roughly: the number of gauge angle points is twice the maximum spin), hence a total of $8,000$ points, each of them with the same computational cost as a regular HFB iteration.

Generator coordinate method - Assume simply two collective coordinates q_1 and q_2. Example: $(q_1, q_2) \equiv (Q_{20}, Q_{22})$ (γ-soft nuclei), (Q_{20}, Q_{30}) (pear-shapes in actinides), etc. If we have 10 points/collective variable, we get a 10^N scaling with the number N of collective variables.

13.4 Exercises

Exercise 44.

Starting from the HFB equation in configuration space, Eq.(13.2), express the HFB equation in coordinate-spin space, Eq.(13.4).

Exercise 45.

Assume a heavy nucleus with axial and triaxial quadrupole, as well as axial octupole degrees of freedom. Suppose you want to calculate the collective excitation spectrum up to spin $I = 20$.

- Based on the estimates above, how many HFB calculations will be needed?
- How many "rotations in gauge space" (including both particle number and Euler angles) are needed?
- Assume we want to use a separable interaction (Gogny-like) and a large basis (why?) so that we use 8 MPI tasks/HFB calculation, and 4 OpenMP threads/MPI task: how many CPU do you need?

If we want to repeat this exercise for all even-even nucleus that are bound ($\approx 1,000$), how many cores do we need?

Lecture 14

Open questions in nuclear DFT [Week 3, day 4]

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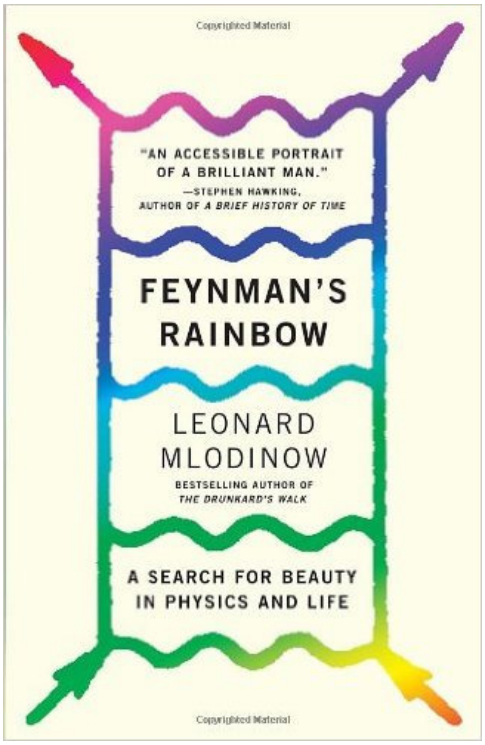
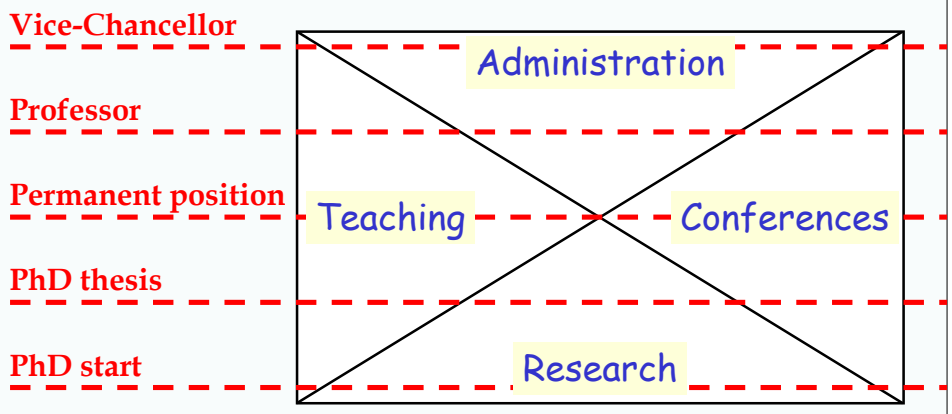
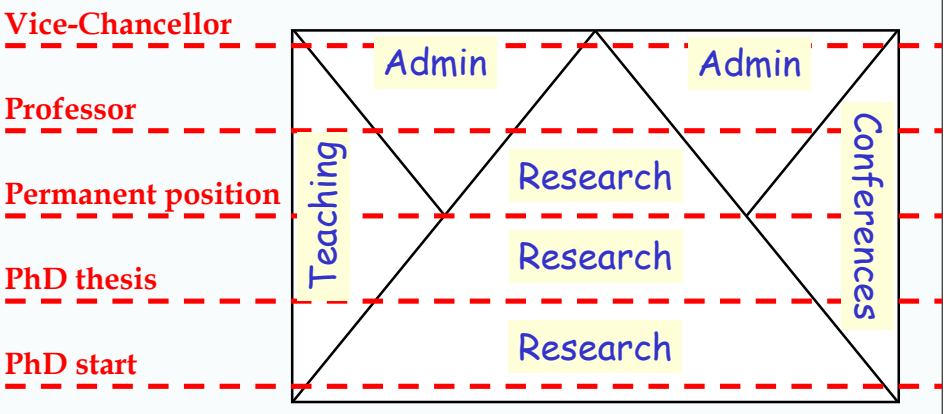


Figure 14.1: Feynman's Rainbow: A Search for Beauty in Physics and in Life, by Leonard Mlodinow [46].

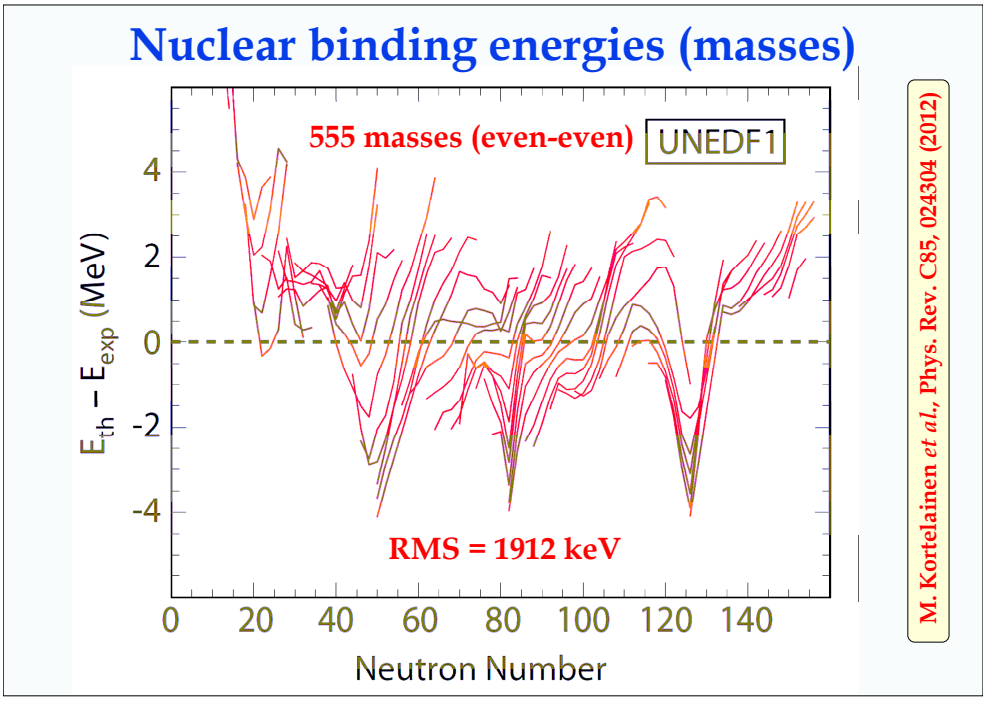
Scientist's envelope of life

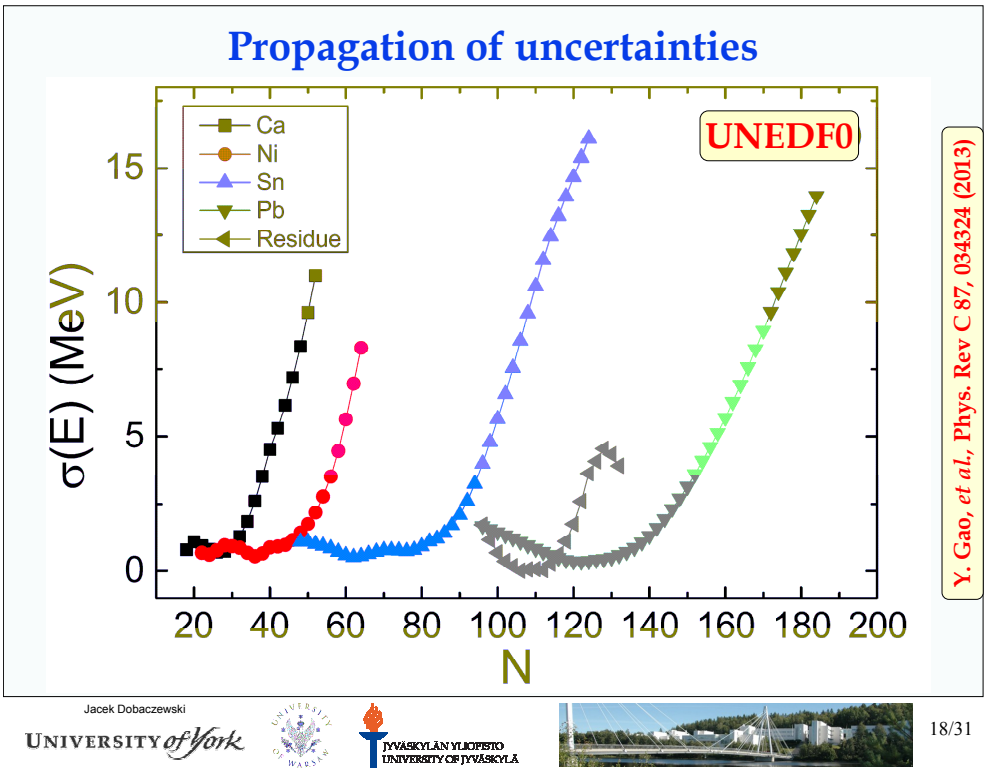


Scientist's envelope of life (maybe yours?)



14.1 Precision frontier

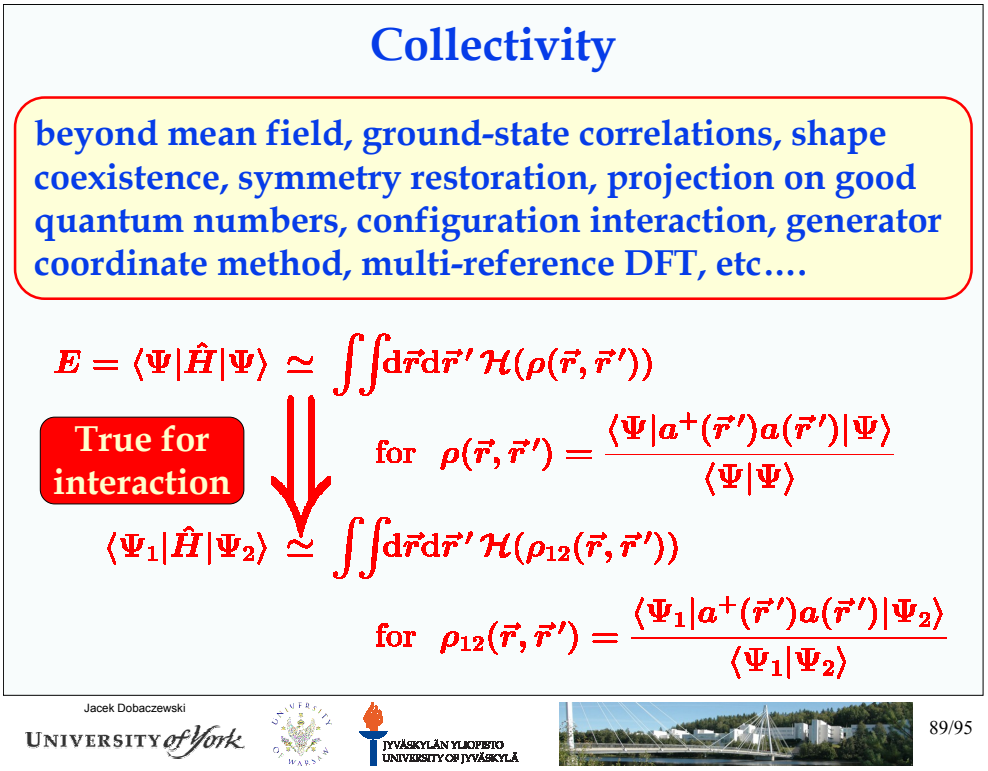




1) **"Remember that all models are wrong; the practical question is how wrong do they have to be to not be useful"**
G.E.P. Box and N.R. Draper
Empirical Model Building and Response Surfaces
(John Wiley & Sons, New York, 1987)

- Error Estimates of Theoretical Models: a Guide:
  J. Dobaczewski, W. Nazarewicz, P.-G. Reinhard,
  J. Phys. G: Nucl. Part. Phys. 41 (2014) 074001
- Enhancing the interaction between nuclear experiment and theory through information and statistics
  D.G. Ireland and W. Nazarewicz
  J. Phys. G: Nucl. Part. Phys. 42 (2015) 030301

14.2 Density functionals for matrix elements



In order to bring forward the origin of singularities in energy kernels [47, 48, 49], it is instructive to recall principal properties of the standard GWT approach. Let us start with a one-body density-independent operator $\hat{F} = \sum_{ij} F_{ij} a_i^\dagger a_j$. Its off-diagonal kernel (the matrix element divided by the overlap), can be calculated with the aid of GWT, and reads [50]:

$$\frac{\langle\Psi|\hat{F}|\tilde{\Psi}\rangle}{\langle\Psi|\tilde{\Psi}\rangle} = \sum_{ij} F_{ij}\,\overline{a_i^+ a_j} \equiv \sum_{ij} F_{ij}\tilde{\rho}_{ji}, \tag{14.1}$$

where

$$\tilde{\rho}_{ji} \equiv \overline{a_i^+ a_j} \equiv \frac{\langle\Psi|a_i^+ a_j|\tilde{\Psi}\rangle}{\langle\Psi|\tilde{\Psi}\rangle}, \tag{14.2}$$

denotes transition density matrix. Therefore, its matrix element between the unprojected state $|\Psi\rangle$ and AMP state $|IMK\rangle = \hat{P}^I_{MK}|\Psi\rangle$ can be calculated from

$$\begin{aligned} F_{IMK} &\equiv \langle\Psi|\hat{F}\hat{P}^I_{MK}|\Psi\rangle \\ &= \frac{2I+1}{8\pi^2}\int d\Omega\, D^{I\star}_{MK}(\Omega)\langle\Psi|\hat{F}|\tilde{\Psi}\rangle, \end{aligned} \tag{14.3}$$

where

$$\hat{P}^I_{MK} = \frac{2I+1}{8\pi^2}\int D^{I*}_{MK}(\Omega)\hat{R}(\Omega)\,d\Omega \tag{14.4}$$

is the AMP operator, $D^I_{MK}(\Omega)$ is the Wigner function, and $\hat{R}(\Omega) = e^{-i\alpha\hat{I}_z}e^{-i\beta\hat{I}_y}e^{-i\gamma\hat{I}_z}$ stands for the active rotation operator in space, parametrized in terms of Euler angles $\Omega = (\alpha, \beta, \gamma)$,

and M and K denote the angular-momentum components along the laboratory and intrinsic z-axis, respectively [51, 52].

The immediate conclusion stemming from Eqs. (14.1)–(14.2) is that the overlaps, which appear in the denominators of the matrix element and transition density matrix, cancel out, and the matrix element $\langle\Psi|\hat{F}|\tilde{\Psi}\rangle$ of an arbitrary one-body density-independent operator $\hat{F}$ is free from singularities and can be safely integrated, as in Eq. (14.3).

Let us now turn our attention to two-body operators. The most popular two-body effective interactions used in nuclear structure calculations are the zero-range Skyrme [53, 54] and finite-range Gogny [55] effective forces. Because of their explicit density dependence, they should be regarded, for consistency reasons, as generators of two-body part of the nuclear EDF. The transition matrix element of the two-body generator reads:

$$\langle\Psi|\hat{V}_{\rm 2B}|\tilde{\Psi}\rangle = \frac{1}{4}\sum_{ijkl}\bar{V}_{ijkl}\left[\tilde{\rho}\right]\ \langle\Psi|a_i^+a_j^+a_la_k|\tilde{\Psi}\rangle, \tag{14.5}$$

where $\bar{V}_{ijkl}\left[\tilde{\rho}\right]$ denotes the antisymmetrized transition-density-dependent matrix element. Gogny and Skyrme effective interactions both contain local terms proportional to ρ^η which, in the MR DFT formulation, are usually replaced with the transition (mixed) density $\rho^\eta \to \tilde{\rho}^\eta$ [56]. Such a procedure, although somewhat arbitrary, is very common, because it fulfills a set of internal consistency criteria formulated in Refs. [57, 58]. These include hermiticity, independence of scalar observables on the orientation of the intrinsic system, and consistency with the underlying mean field. The alternative way of proceeding is to substitute density-dependent terms with projected density [59] or average density [60]. These scenarios do not fulfill all the consistency criteria and will not be discussed here.

Evaluating the transition matrix element, Eq. (14.5), with the aid of GWT, one obtains,

$$\begin{aligned}\frac{\langle\Psi|\hat{V}_{\rm 2B}|\tilde{\Psi}\rangle}{\langle\Psi|\tilde{\Psi}\rangle} &= \frac{1}{4}\sum_{ijkl}\bar{V}_{ijkl}\left[\tilde{\rho}\right]\ \Big(\overbrace{a_i^+a_j^+}\ \overbrace{a_la_k}\\ &+ \overbrace{a_i^+a_k}\ \overbrace{a_j^+a_l} - \overbrace{a_i^+a_l}\ \overbrace{a_j^+a_k}\Big).\end{aligned} \tag{14.6}$$

Furthermore, for particle-number-conserving theory, contractions $\overbrace{a_i^+a_j^+}$ and $\overbrace{a_la_k}$ vanish, whereas the remaining two contractions give products of two transition density matrices,

$$\frac{\langle\Psi|\hat{V}_{\rm 2B}|\tilde{\Psi}\rangle}{\langle\Psi|\tilde{\Psi}\rangle} = \frac{1}{4}\sum_{ijkl}\bar{V}_{ijkl}\left[\tilde{\rho}\right]\ \left(\tilde{\rho}_{ki}\tilde{\rho}_{lj} - \tilde{\rho}_{li}\tilde{\rho}_{kj}\right), \tag{14.7}$$

or

$$\begin{aligned}\frac{\langle\Psi|\hat{V}_{\rm 2B}|\tilde{\Psi}\rangle}{\langle\Psi|\tilde{\Psi}\rangle} &= \frac{1}{4}\sum_{ijkl}\bar{V}_{ijkl}\left[\tilde{\rho}\right]\ \left(\frac{\langle\Psi|a_i^+a_k|\tilde{\Psi}\rangle\ \langle\Psi|a_j^+a_l|\tilde{\Psi}\rangle}{\langle\Psi|\tilde{\Psi}\rangle^2}\right.\\ &- \left.\frac{\langle\Psi|a_i^+a_l|\tilde{\Psi}\rangle\ \langle\Psi|a_j^+a_k|\tilde{\Psi}\rangle}{\langle\Psi|\tilde{\Psi}\rangle^2}\right),\end{aligned} \tag{14.8}$$

that is, the transition matrix element reads

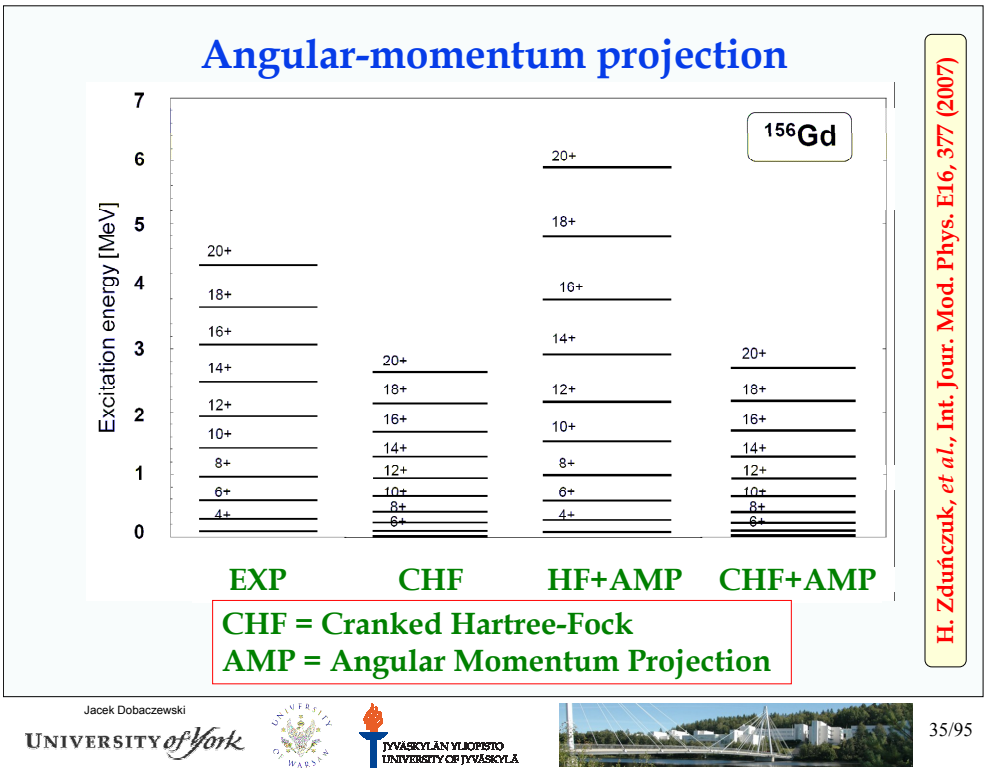
$$\langle\Psi|\hat{V}_{\rm 2B}|\tilde{\Psi}\rangle = \frac{1}{2}\sum_{ijkl}\bar{V}_{ijkl}\left[\tilde{\rho}\right]\ \frac{\langle\Psi|a_i^+a_k|\tilde{\Psi}\rangle\ \langle\Psi|a_j^+a_l|\tilde{\Psi}\rangle}{\langle\Psi|\tilde{\Psi}\rangle}. \tag{14.9}$$

This defines the matrix element between the unprojected and AMP states,

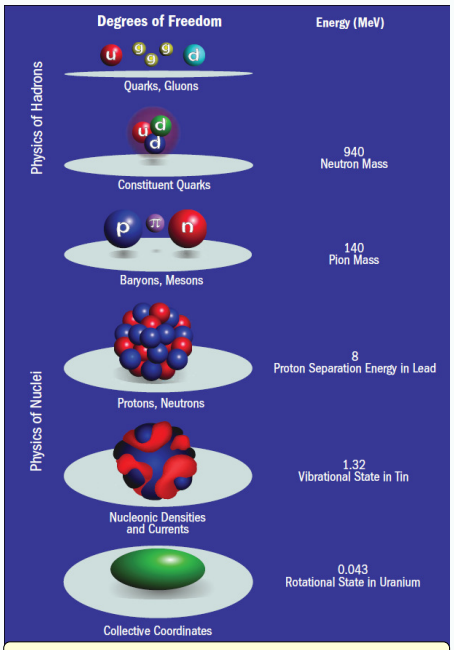
$$V^{\rm 2B}_{IMK} \;=\; \frac{2I+1}{8\pi^2}\int d\Omega\, D^{I\,\star}_{MK}(\Omega)\langle\Psi|\hat{V}_{\rm 2B}|\tilde{\Psi}\rangle. \tag{14.10}$$

We note here that, because of the density dependence of the two-body interaction, the analogue the first member of Eq. (14.3), that is, $V^{\rm 2B}_{IMK} \equiv \langle\Psi|\hat{V}_{\rm 2B}\hat{P}^{I}_{MK}|\Psi\rangle$ is not valid. Nevertheless, expression (14.10) constitutes a consistent definition of the matrix element.

At variance with the one-body case discussed above, the integrand in Eq. (14.10) is inversely proportional to the overlap, thus containing potentially dangerous (singular) terms. The singularity disappears only if the sums in the numerator, evaluated at angles Ω where the overlap $\langle\Psi|\tilde{\Psi}\rangle$ equals zero, give a vanishing result; such a cancellation requires evaluating the numerator without any approximations or omitted terms. An additional singularity is created by the density dependence of the interaction.



14.3 Effective theory of the DFT and gradient expansions



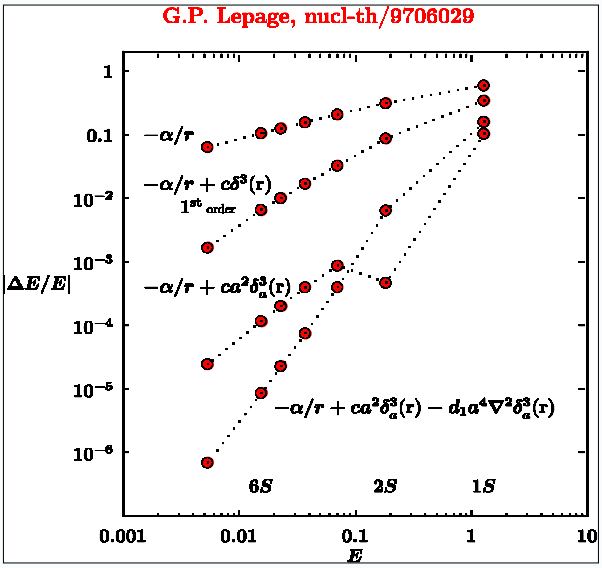
G.F. Bertsch, *et al.*, Scidac Review 6, 42 (2007)

- An effective theory (ET) is a theory which "effectively" captures what is physically relevant in a given domain.
- The most appropriate description of particle interactions in the language of quantum field theory (QFT) depends on the energy at which the interactions are studied.
- Objective reductionism (Weinberg): the convergence of arrows of scientific explanation.
- Emergence (Anderson): "at each new level of complexity entirely new properties appear and the understanding of the new behaviors requires research which I think is as fundamental in its nature as any other".

Elena Castellani, physics/0101039

Hydrogen atom perturbed near the center

G.P. Lepage, nucl-th/9706029



Relative errors in the S-wave binding energies are plotted versus:
(i) the binding energy for the Coulomb theory
(ii) the Coulomb theory augmented with a delta function in first-order perturbation theory
(iii) the non-perturbative effective theory through a^2, and
(iv) the effective theory through a^4.

We regularize the zero-range delta interaction using the Gaussian function,

$$\delta(\boldsymbol{r}) = \lim_{a\to 0} g_a(\boldsymbol{r}) = \lim_{a\to 0} \frac{e^{-\frac{r^2}{a^2}}}{(a\sqrt{\pi})^3}.$$

Then, the resulting central two-body regularized pseudopotential reads,

$$V(\boldsymbol{r}_1\boldsymbol{r}_2;\boldsymbol{r}'_1\boldsymbol{r}'_2) = \sum_{i=1}^{4} \hat{P}_i\hat{O}_i(\boldsymbol{k}',\boldsymbol{k})\delta(\boldsymbol{r}_1-\boldsymbol{r}'_1)\delta(\boldsymbol{r}_2-\boldsymbol{r}'_2)g_a(\boldsymbol{r}_1-\boldsymbol{r}_2),$$

where $\boldsymbol{k} = \frac{1}{2i}(\boldsymbol{\nabla}_1-\boldsymbol{\nabla}_2)$ and $\boldsymbol{k}' = \frac{1}{2i}(\boldsymbol{\nabla}'_1-\boldsymbol{\nabla}'_2)$ are the standard relative-momentum operators, and the Wigner, Bartlett, Heisenberg, and Majorana terms are given by the standard spin and isospin exchange operators, $\hat{P}_1 \equiv 1$, $\hat{P}_2 \equiv \hat{P}_\sigma$, $\hat{P}_3 \equiv -\hat{P}_\tau$, $\hat{P}_4 \equiv -\hat{P}_\sigma\hat{P}_\tau$.

To give a specific example, up to the second-order, that is, up to the next-to-leading-order (NLO) expansion, operators $\hat{O}_i(\boldsymbol{k}',\boldsymbol{k})$ read

$$\hat{O}_i(\boldsymbol{k}',\boldsymbol{k}) = T_0^{(i)} + \frac{1}{2}T_1^{(i)}\left(\boldsymbol{k}'^{*2}+\boldsymbol{k}^2\right) + T_2^{(i)}\boldsymbol{k}'^{*}\cdot\boldsymbol{k},$$

where $T_k^{(i)}$ are the channel-dependent coupling constants.

$$V(\boldsymbol{r}_1\boldsymbol{r}_2;\boldsymbol{r}'_1\boldsymbol{r}'_2) = \sum_{i=1}^{4} \hat{P}_i\hat{O}_i(\boldsymbol{k}',\boldsymbol{k})\delta(\boldsymbol{r}_1-\boldsymbol{r}'_1)\delta(\boldsymbol{r}_2-\boldsymbol{r}'_2)g_a(\boldsymbol{r}_1-\boldsymbol{r}_2),$$

$$\hat{O}_i(\boldsymbol{k}',\boldsymbol{k}) \;=\; \sum\nolimits_{nj} T_j^{(ni)}\hat{O}_j^{(n)}(\boldsymbol{k}',\boldsymbol{k})$$

Differential operators $\hat{O}_j^{(n)}(\boldsymbol{k}',\boldsymbol{k})$ are scalar polynomial functions of two vectors, so owing to the Generalized Cayley-Hamilton theorem, they must be polynomials of three elementary scalars: $\boldsymbol{k}^2$, $\boldsymbol{k}'^2$, and $\boldsymbol{k}'\cdot\boldsymbol{k}$, or

$$\hat{T}_1 \;=\; \tfrac{1}{2}(\boldsymbol{k}'^{*2}+\boldsymbol{k}^2), \quad \hat{T}_2 = \boldsymbol{k}'^{*}\cdot\boldsymbol{k}, \quad \hat{T}_3 = \tfrac{1}{2}(\boldsymbol{k}'^{*2}-\boldsymbol{k}^2),$$

with the condition that only even powers of $\hat{T}_3$ can appear. In terms of $\hat{T}_1$, $\hat{T}_2$, and $\hat{T}_3$, we now can define the following differential operators:

$$\begin{aligned}
\text{LO:}\quad & \hat{O}_1^{(0)}(\boldsymbol{k}',\boldsymbol{k}) &&= \hat{1}, \\
\text{NLO:}\quad & \hat{O}_1^{(2)}(\boldsymbol{k}',\boldsymbol{k}) &&= \hat{T}_1, \quad \hat{O}_2^{(2)}(\boldsymbol{k}',\boldsymbol{k}) = \hat{T}_2, \\
\text{N2LO:}\quad & \hat{O}_1^{(4)}(\boldsymbol{k}',\boldsymbol{k}) &&= \hat{T}_1^2+\hat{T}_2^2, \quad \hat{O}_2^{(4)}(\boldsymbol{k}',\boldsymbol{k}) = 2\hat{T}_1\hat{T}_2, \\
& \hat{O}_3^{(4)}(\boldsymbol{k}',\boldsymbol{k}) &&= \hat{T}_1^2-\hat{T}_2^2, \quad \hat{O}_4^{(4)}(\boldsymbol{k}',\boldsymbol{k}) = \hat{T}_3^2.
\end{aligned}$$

We performed derivations of average energies separately for all terms of the regularized finite-range pseudopotential. The final result of this derivation is given by linear combinations of terms of the EDF appearing on the rhs of the following expression,

$$\langle C^{\tilde{n}'\tilde{L}',\tilde{t}}_{\tilde{n}\tilde{L},v_{12}\tilde{S}}\hat{V}^{\tilde{n}'\tilde{L}',\tilde{t}}_{\tilde{n}\tilde{L},v_{12}\tilde{S}}\rangle = \sum C^{a',\alpha',t,\mathcal{L}}_{a,\alpha,Q}T^{a',\alpha',t,\mathcal{L}}_{a,\alpha,Q}.$$

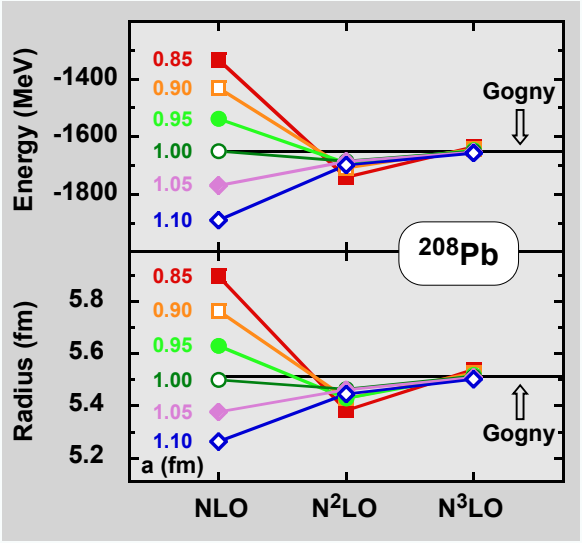
In this expression, $C^{a',\alpha',t,\mathcal{L}}_{a,\alpha,Q}$ and $T^{a',\alpha',t,\mathcal{L}}_{a,\alpha,Q}$ denote, respectively, the coupling constants and terms of the EDF according to the compact notation, where the Greek indices $\alpha = \{n_\alpha S_\alpha v_\alpha J_\alpha\}$ and Roman indices $a = \{m_a I_a\}$ combine all the quantum numbers of the local densities $\rho_\alpha(\boldsymbol{r})$ and derivative operators D_a in the spherical-tensor formalism, that is,

$$T^{a',\alpha',t,L}_{a,\alpha,Q} = \int \mathrm{d}\boldsymbol{r}_1 \mathrm{d}\boldsymbol{r}_2 \, g_a(\boldsymbol{r}) \left[\left[\left[D_{a'} \rho^t_{\alpha'}(\boldsymbol{r}_1) \right]_Q \left[D_a \rho^t_\alpha(\boldsymbol{r}_2) \right]_Q \right]^0 \right]_0 .$$

$$T^{a',\alpha',t,N}_{a,\alpha,Q} = \int \mathrm{d}\boldsymbol{r}_1 \mathrm{d}\boldsymbol{r}_2 \, g_a(\boldsymbol{r}) \left[\left[\left[D_{a'} \rho^t_{\alpha'}(\boldsymbol{r}_1, \boldsymbol{r}_2) \right]_Q \left[D_a \rho^t_\alpha(\boldsymbol{r}_2, \boldsymbol{r}_1) \right]_Q \right]^0 \right]_0 ,$$

They have been obtained using the integration by parts to transfer all derivatives onto the density matrices, and then employing the locality deltas to perform integrations over two out of four space coordinates.

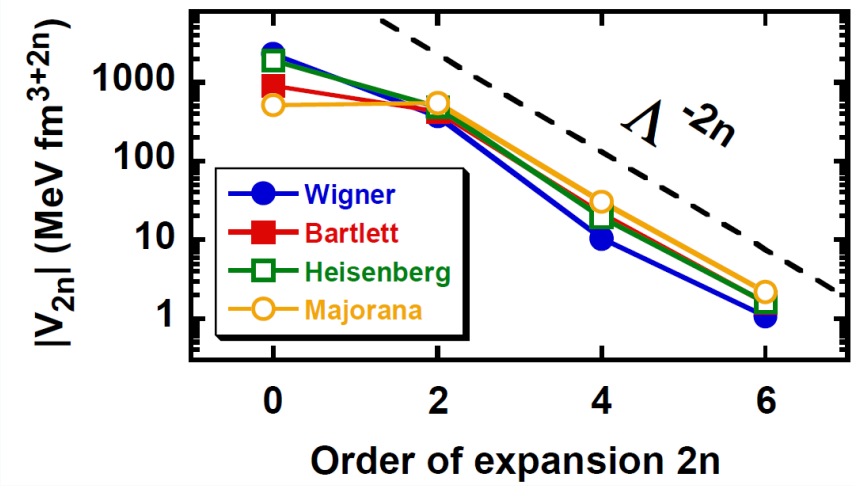
Regularized pseudopotentials vs. Gogny



J.D, K. Bennaceur, F. Raimondi, J. Phys. G. 39, 125103 (2012)

Coupling constants of the regularized pseudopotentials

$\Lambda \approx 700$ MeV/$\hbar c \approx 3.8$ fm^{-1}



J.D, K. Bennaceur, F. Raimondi, J. Phys. G. 39, 125103 (2012)

14.4 Large-scale Calculations

14.4.1 Fission

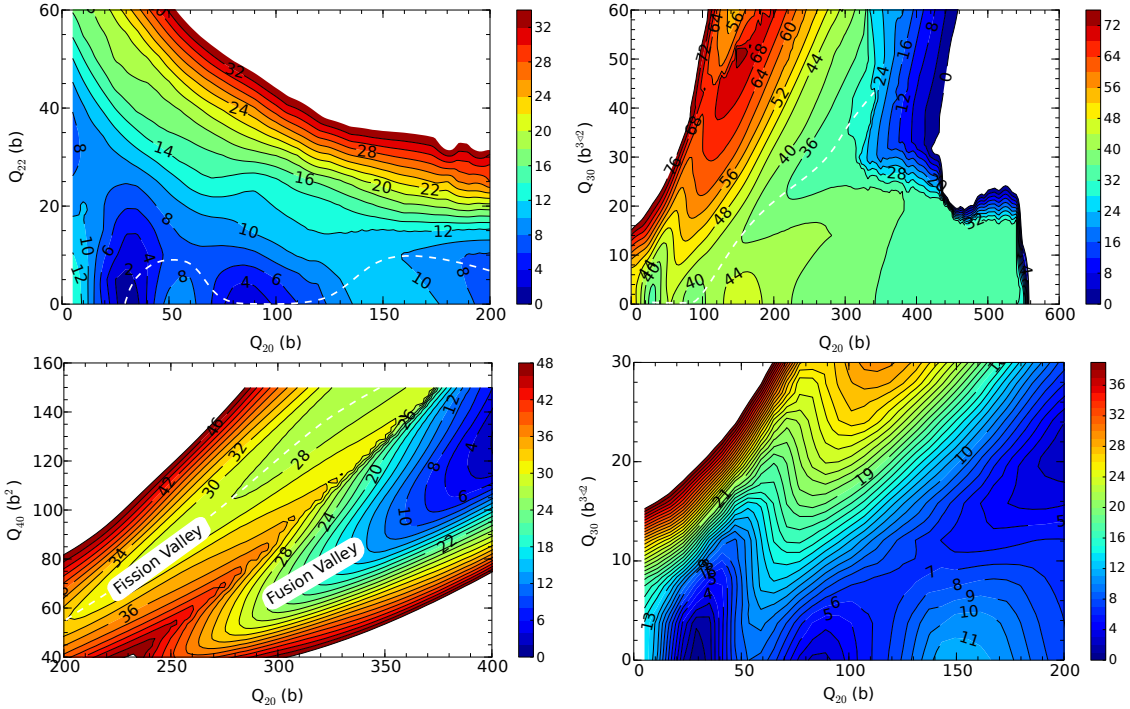


Figure 14.2: N. Schunck, D. Duke, H. Carr, and A. Knoll, [61].

14.4.2 Multi-reference EDF

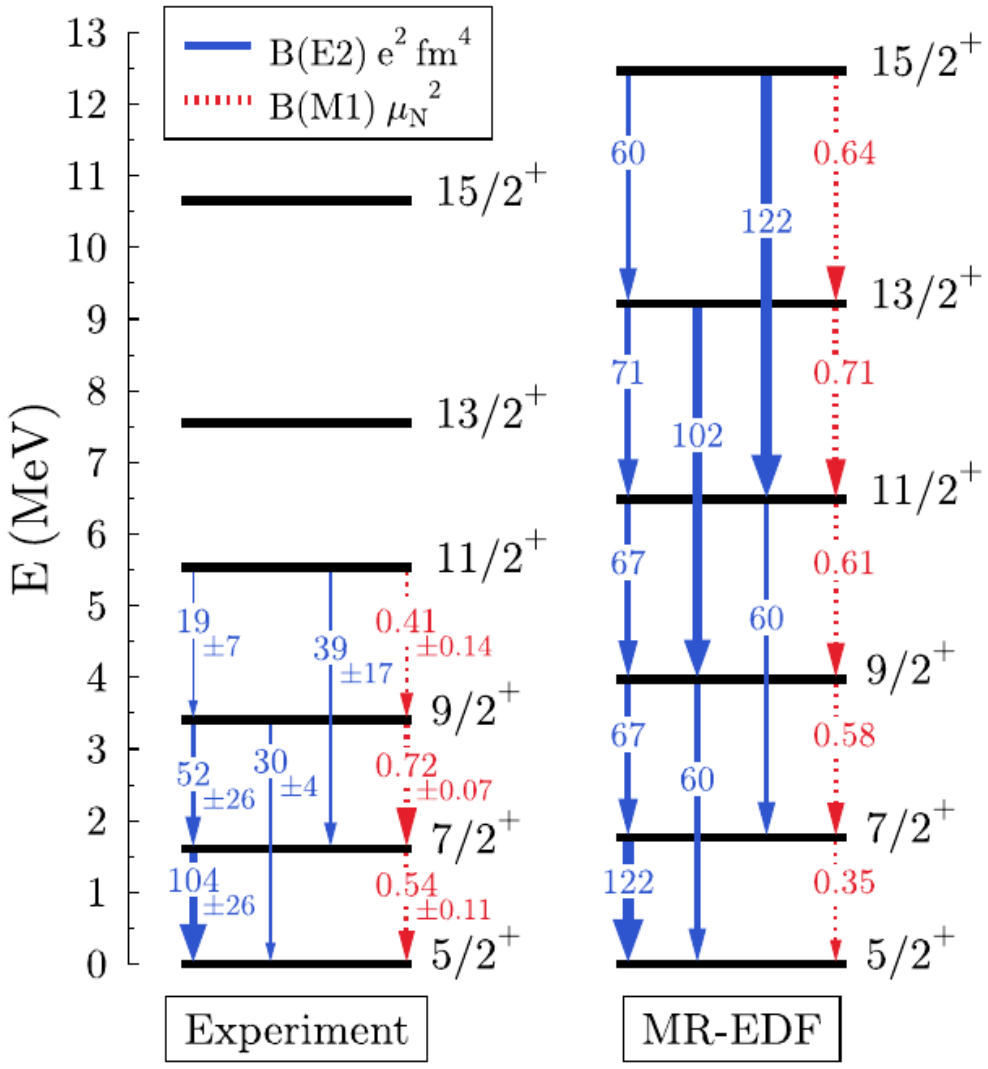


Figure 14.3: Excitation energies of states in the ground-state band of ^{25}Mg, and B(E2) and B(M1) values for transitions between them. B. Bally, B. Avez, M. Bender, and P.-H. Heenen, [62].

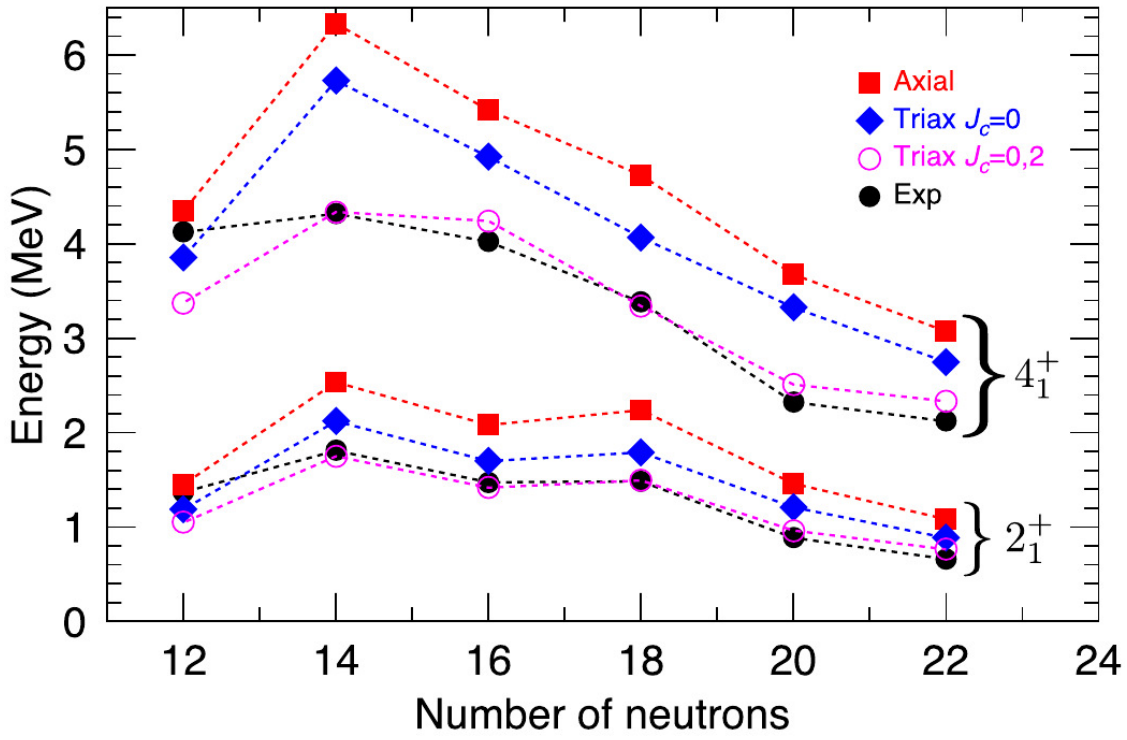
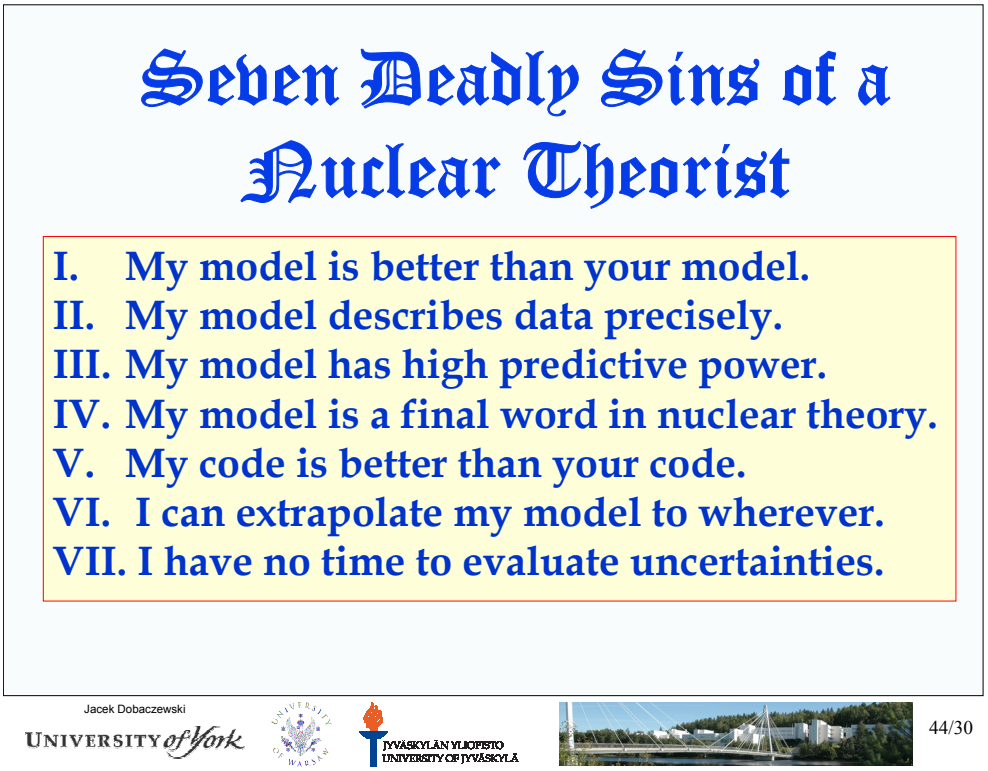


Figure 14.4: 2^+ and 4^+ excitation energies for the Mg isotopic chain calculated with the GCM method including axial states (red squares), axial+triaxial with $J_c = 0$ states (blue diamonds) and axial+triaxial with $J_c = 0, 2$ states (magenta open dots). M. Borrajo, T.R. Rodriguez, and J.L. Egido, [63].

14.5 Take-away messages

- Read current publications. Follow the arXiv. Participate in (or request) a journal club.
- Talk to experimentalists.
- Avoid traps.



Lecture 15

Students' questions [Week 3, day 5]

1. (a) "Why does DFT work "better" (model more accurately phenomena) in some fields of research than in others? " For example, modelling electrons seems to be far simpler and more is known about it than applying DFT to nucleons when they are all fermions. I guess it has to do with the strong force and QCD more generally but it would be nice to get a little more detail on what the specific challenges are and why these challenges don't apply to every case of DFT.

   and closely connected to this,

   (b) "What, if any, are the applications of the theory currently and what potential applications do you believe it could have in the future, both in theoretical and experimental physics (and possibly wider society/industry)? "

2. What would be necessary for DFT to achieve the same level of accuracy/precision as experiment? Is it bigger computers, more sophisticated functionals, a more general theory? Or is it a fool's errand?

3. my question regards the separation of the energy functional (for example in Skyrme theory) in isospin, isovector, time-even and time-odd part:

   I would like to have a remarks about the properties of the nucleus (symmetries and experimental observables) that can be related to the different parts.

   The idea is to clarify me in which sector of the functional is necessary to work in order to improve its predictive power.

4. I know Nicolas mentioned that HFB could be used for excited states as well as ground states (by acting on the HFB ground state with some quasiparticle operator, I think). In practice, what information does that give us? Can we extract single particle excitations, or collective nuclear excitations, or just quasiparticle excitations?

5. "How can I verify that given multipole moment operators make sense? What physical properties can I find by applying these operators on a state describing a nucleus?"

6. 1) How exactly the case of even-odd and odd-odd nuclei is handled in DFT framework (blocking method...)

   2) As we know density dependence of the coupling constant is needed to reproduce saturation density. This lead to spuriousity while restoring symmetry. Is there any systematic way to construct a spuriosity-free functional ? (Inclusion of a3-body terms etc...)

7. During the course we have discussed phenomenological functionals and the fact that for each different parametrisation of a such functionals an adjustment on experimental data is needed. Hence, to what extend can new experimental measurements of exotic systems actually help in improving or constrain such functionals? I also have another question closely related to the first one. Providing that new experimental values can actually help in further constraining the different functionals, at present do you have any idea on what observables would bring the most stringent constraints?

8. I don't know if this question is fully inside of the DFT theory we have seen, but I am curious about the topic. It is about the fitting of the phenomenological nuclear functionals.

   I was wondering how the values of the constants of the phenomenological potentials (t0, t1, t2, t3, x0, x1, x2, x3, W0 for Skyrme, Hi, Wi, Bi, Mi, t3,x3, W0 for Gogny, etc.) are fitted. That is to say, usually to which parameters are these interactions fitted? Are mostly experimental values or can the parameters be fixed by hand in order to reproduce a certain behaviour? How to choose which parameters use? And in general, how is the process of the fitting? Do you have to take into account anything special?

   I am currently working with symmetry energies when studying neutron stars, and it is seen that they tend to have similar values at low densities, meanwhile at larger densities the behabiour between the different fittings is different, I supose because at larger densities one does not have parameters to fit and then one has to extrapolate.

But could it be some kind of constraint/parametrization in order to have better behaviours at larger densities? How is this behaviour at larger densities treated in the process of fitting (if it is considered)?

9. I want to know more details about BCS model and Bogoliubov transformation. Both BCS and HFB include the concept of quansipaticle. BCS ground state is HFB vacuum. I want to know the essential difference of these two methods and something about quasipaticle.

10. The question is about the interpretation of broken symmetries, restored symmetries and what does a nucleus "really" look like. The symmetry-breaking solution of mean-field equations, according to notes, should be interpreted as an approximation of the wave packet and not of a true nuclear eigenstate. As I understand, this should be just the consequence of the fact that this state - not having the good quantum number of the broken symmetry - actually corresponds to a linear combination (wave packet) of states with different good quantum numbers. For example, my pear-shaped Ba144 nucleus on a mean-field level corresponds to a mixture of states with positive and negative parity and does not correspond to a nuclear state which can be directly measured in experiment. By restoring symmetries ("going back to a laboratory frame") we obtain states with either positive or negative parity which can actually be directly measured, alongside with transitional properties between them. Therefore, when we say that we have measured a nucleus to be pear-shaped, this is truly an imagination: nucleus as we measure it can never be pear-shaped since all of its eigenstates have good parity. What we have actually discovered is that the eigenstates of the nucleus can be used to build a wave packet which will, for example, have non-vanishing expectation value of octupole moment operator (this value will come precisely from the large off-diagonal elements that we have measured; all diagonal elements should give zero). However, outside of our apparatus nothing prevents nucleus to be in precisely this wave packet state - therefore, the nucleus can indeed and for real be pear-shaped.

    After long discussion, my questions would be:

    1. Is my reasoning correct? If yes, is this kind of wave packets somehow treated theoretically? What is their connection with interpreted wave packets from a MF level?

    2. How can this kind of reasoning be extended to the case of spherical symmetry-breaking quadrupole-deformed nuclei? Are "pancake" and "cigar" shapes any more or less real than pears? (Of course, I

know they are way more common.)

11. 1. How EDFs are fit, what are the quantities people care (most) about when fitting, and why (what are the importance of these quantities)?

    2. Are there quantities that work against each other (for e.g. if I want to get a better overall radius fit Ill have to sacrifice mass)?

    3. When doing a mass table calculation, why cant we choose different EDFs for the region that they are good at and mix the result together, and usually (what I know of) use a single EDF?

    4. A few comments (or point a direction, references) about how to productively analyze uncertainty when using EDFs

12. With recent advances in the development of accelerator cards (Intel phi or GPUs), do you see any benefit to be had in (TD)DFT codes from using them? The newest generations have more and more local memory on the board, requiring less data transfer, but I suppose the problem may not scale well. Thoughts?

13. "What is the uncertainty of the DFT method? What gives the largest contribution to it: the unknown form of the true functional, the fit of the parameters, the numerical errors of computing methods or something else?"

14. What are the main observed phenomena in experiments that the nuclear theory can't or has difficulties to reproduce?

15. How is the performance and validity of using a DME-treated density functional compared to using an 'exact' one in HF calculations?

16. Two questions come to mind, and I don't know which one of them, if any, would be more applicable. So, you can choose which one will be discussed.

    First, can something like the Bogoliubov transformation be used to treat phenomena like alpha clustering? If so, is there something analogous to the BCS approximation in that case?

    Second, what happens with pairing when nuclei have nonzero temperature? Naively we would expect BCS to not work at one point because it's like superfluidity and that gets destroyed at sufficiently large temperatures. Does the same happen in the full H(F)B treatment? Are there any kinds of pairing that BCS can not

qualitatively describe?

The question I want to ask the most is if there is any way to extend mean-field theories so that mesons are treated as real constituents of nuclei instead of just appearing as classical fields, but I suspect answering that would take three more weeks at least.

17. One question I ask myself is about hfb+gcm. If we considere a state |hfbgcm> = f_i \prod_j \gamma_{ij} |0> and we minimize directly the energy of |hfbgcm> with constraints on each \prod_j\gamma_{ij}|0>, so we calculate hfb states at the same time than the gcm state, we can think that the result will be better than with calculations of hfb states and then gcm. There is any work on this ? Which kind of correlation can we obtain?

18. In your famous paper published in 1984, you introduced abnormal density \quad \rho to replace pairing tensor which appears in standard HFB theory. Can you explain their relationship in details and why you introduced them? Just for convenience in computation or other deep reasons?

    And I am not sure whether such specific question is suited for discussion class. If not, I would like to discuss something about Goldstein theorem in spontaneous symmetry broken because even I read the lecture, I know nothing about what the theorem express.

19. Can we predict beta decay and alpha decay based on DFT?
    If we can, is it only to create excited states, and calculate the transition matrix element? Or need something correction?

20. We spoke a bit about asymmetric kernels/matrix elements in the case of MR-EDF and on a broader picture for symmetry breaking and restoration, but are there other cases in which those have been shown to be useful/necessary?

21. Given that there are hundreds (thousands?) of functionals to choose from, how do we make the decision of which one to use for a given physical problem? Are there some functionals which are definitely better than others? Are there some which should never be used?

22. Just today, you said something about the impossibility of doing calculations beyond mean field with two-body potentials that include density dependence. First of all, I didn't understand the reason of that. Moreover, this should means that we are not able to expand the terms that correspond to the three body interaction after the first order of perturbation: is it an important limitation of the model?

23. In fig 14.4 in lecture notes, between N=12 and N=14, it seem that all

three theoretical lines have higher slope compared to the experimental result. Can this difference be explained with some physics argument?

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