Nuclear Physics 30

The mean-field potential:

Hartree-Fock, Skyrme,

Gogny and all that

RECAP

Shell-model → two problems

1) How to find a good V^{MF} ?

1.a) Convenient
(Oscillator potential)

1.b) Other more theoretical means (Hartree-Fock)

↓

TODAY'S LESSON

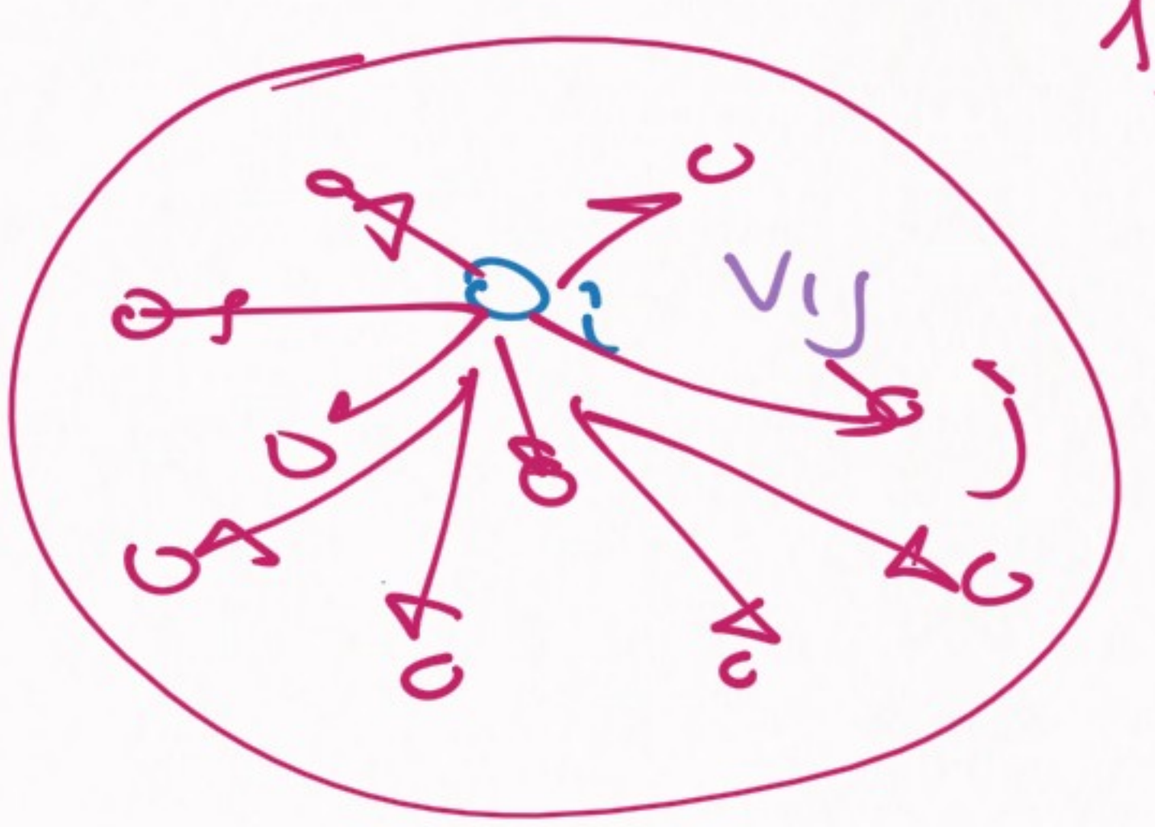
2) How to deal with residual interaction ?

↓

PAST LESSON

Today → MEAN FIELD POTENTIAL

Basic idea :



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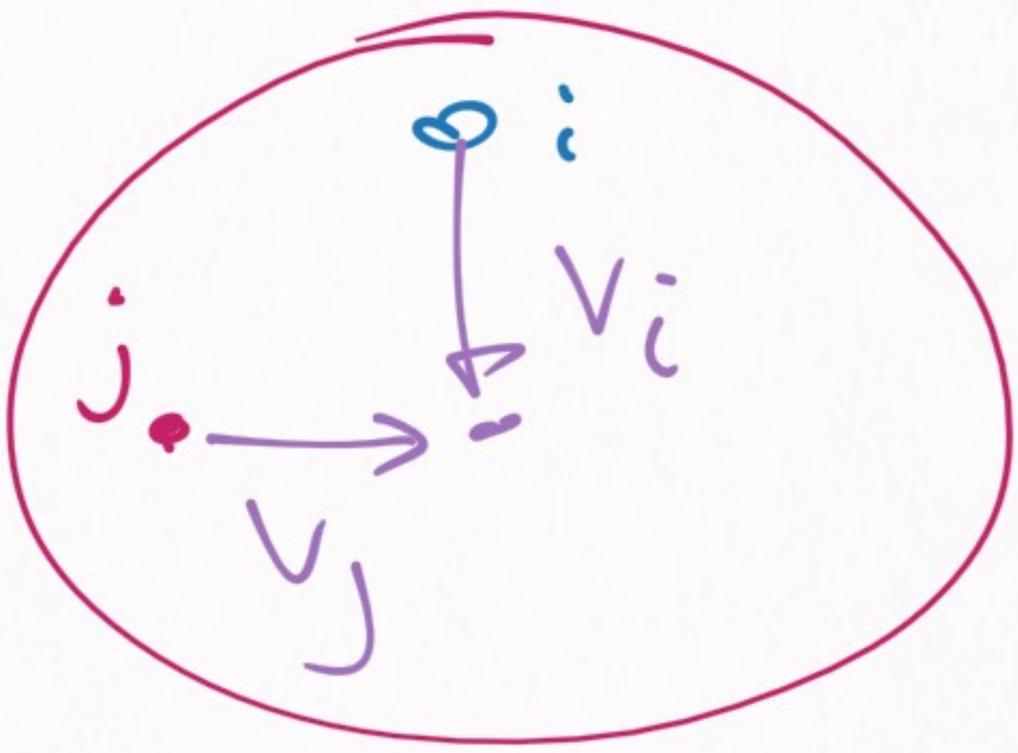
1) Each particle affects each other

We average



1) Each particle feels an average potential

THE MEAN FIELD POTENTIAL

How to derive it?

→ GOD'S VIEW

1) We have the A-body Schrödinger equation

$$\left(\sum_i T_i + \sum_{ij} V_{ij}\right)\Psi(\vec{r}_1 \dots \vec{r}_A) = E_A \Psi(\vec{r}_1 \dots \vec{r}_A)$$

We solve it for some V_{ij} and obtain the A-body wave function

2) For each particle, we get the average potential

$$V_i(\vec{r}_i) = \sum_{j \neq i} \int (\prod_{j \neq i}) d^3\vec{r}_j$$

$$\times |\Psi_A(\ldots \vec{r}_i \ldots \vec{r}_j \ldots)|^2 V(\vec{r}_i - \vec{r}_j)$$

Or, more elegantly:

$$\hat{V}_i(\vec{r}) = \delta(\vec{r} - \vec{r}_i) \sum_{j \neq i} V(\vec{r}_i - \vec{r}_j)$$

$$V_i(\vec{r}) = \langle \Psi_A | \hat{V}_i(\vec{r}) | \Psi_A \rangle$$

And now we have the average potential V_i

3) Now we can solve

the monoparticular WF's:

$$\left[-\frac{\nabla_i^2}{2m_i} + V_c(\vec{r}_i)\right]\phi_c(\vec{r}_i) = \epsilon_c \phi(\vec{r}_i)$$

4) Find the mean-field A-body

wave function

$$\Psi_A^{MF} = \prod_i \phi_i(\vec{r}_i)$$

Simplification: no anti-symmetrization

But this is sort of idiotic ...

If I can solve the full

A-body wave function,

why do MF approximation?

THE (PROBABLE) REAL SITUATION

1) I have a two-body potential

$$V_{ij} = V(\vec{r}_i - \vec{r}_j)$$

but I can't solve the A-body Schrödinger equation:

$$\left(\sum_i T_i + \sum_{ij} V_{ij}\right)\Psi = E_A \Psi$$

2) So I invent some one-body "mean field" potential

$$V_i^{(0)} = V^{(0)}(\vec{r}_i)$$

$$(T_i + V_i^{(0)})\,\phi_i^{(0)} = \epsilon_i^{(0)}\,\phi_i^{(0)}$$

3) I use the MF wavefunction to obtain a new MF potential

$$\Psi_A^{(0)} = \prod_i \phi_i^{(0)}(\vec{r}_i)$$

$$V_i^{(1)}(\vec{r}) = \langle \psi_A^{(0)} | \hat{V}_i(\vec{r}) | \psi_A^{(0)} \rangle$$

$$\hat{V}_i(\vec{r}) = \delta(\vec{r} - \vec{r}_i) \sum_{j \neq i} V(\vec{r}_i - \vec{r}_j)$$

$$V_i^{(1)}(\vec{r}) = \sum_{j \neq i} |\phi_j^{(0)}|^2 V(\vec{r} - \vec{r}_j)$$

4) I solve again the monoparticular MFs

$$[T_i + V_i^{(1)}(\vec{r})]\phi_i^{(1)}(\vec{r}) = \epsilon_i^{(1)}\phi_i^{(1)}(\vec{r})$$

5) I check if this makes sense:

[$\phi_i^{(0)}(\vec{r}) \simeq \phi_i^{(1)}(\vec{r})$?]

→ Actually this is an iterative algorithm:

$$\left[T_i + V_i^{(n)}\right]\phi_i^{(n)} = \epsilon_i^{(n)}\phi_i^{(n)}$$

$$V_i^{(n+1)} = \sum_{j\neq i}\int d^3\vec{r}_j\,|\phi_j^{(n)}|^2 V(\vec{r}_i - \vec{r}_j)$$

$$\left[T_i + V_i^{(n+1)}\right]\phi_i^{(n+1)} = \epsilon_i^{(n+1)}\phi_i^{(n+1)}$$

And we do this till:

$$\boxed{\phi_i^{(n+1)} \underline{\simeq} \phi_i^{(n)}}$$

THIS IS HARD WORK !!

$\phi^{(n+1)} = \phi^{(n)}$ $\Rightarrow$ Self-consistent calculation

But we made a simplification :

1) Non-identical particles

$$\phi_A = \prod_j \phi_j(\vec{r}_j)$$

$$V_i(\vec{r}_i) = \sum_{j \neq i} \int d3\vec{r}_j \, |\phi_j(\vec{r}_j)|^2 V(\vec{r}_i - \vec{r}_j)$$

$\rightarrow$ With identical particles this will change

2) Identical particles:

$$\Psi_A = \mathcal{A}\left[\prod_j \phi_j(r_j)\right] \quad \text{(fermions)}$$

$$\text{or} \quad S\left[\prod_j \phi_j(r_j)\right] \quad \text{(bosons)}$$

$$\Big[T_i + \sum_{j\neq i} \int d^3\vec{r}_j \, |\phi_j(\vec{r}_j)|^2 V(\vec{r}-\vec{r}_j)\Big]\phi_i(\vec{r})$$

$$\Big[\pm \sum_{j\neq i} \int d^3\vec{r}_j \, \phi_j^*(\vec{r}_j)\,\phi_j(\vec{r})\, V(\vec{r}-\vec{r}_j)\,\phi_i(\vec{r}_j)\Big]$$

$$= \epsilon_i \phi_i(\vec{r})$$

$+ \rightarrow$ bosons

$- \rightarrow$ fermions

difficult

Actually, what we have obtained is a non-local potential:

$$\left[-\frac{\nabla^2}{2m_i}\phi_i(\vec{r}) + \int d^3\vec{r}'\, V_i(\vec{r},\vec{r}')\phi_i(\vec{r}')\right] = \epsilon_i \phi_i(\vec{r})$$

$V_i(\vec{r},\vec{r}')$ → non-local

$$V_i(\vec{r},\vec{r}') = \delta^{(3)}(\vec{r}-\vec{r}') \sum_j \int d^3\vec{r}'\, |\phi_j(\vec{r}')|^2 V(\vec{r}-\vec{r}') - \sum_j \phi_j^*(\vec{r}')\phi_j(\vec{r}) V(\vec{r}-\vec{r}')$$

① ② (circled)

① → HARTREE TERM

② → FOCK TERM

HARTREE-FOCK METHOD

→ Let's try to simplify a bit the previous ideas

$$|\Psi_0\rangle = \mathcal{A}\left[\prod_j \phi_j(r_j)\right]$$

↳ not the full wavefunction

↳ How do we choose a good approximation to this?

↓

Variational principle:

$$\delta\left(\frac{\langle\Psi_0|H|\Psi_0\rangle}{\langle\Psi_0|\Psi_0\rangle}\right) = 0$$

→ $|\Psi_0\rangle$ minimizes the energy

RECAP → Variational principle

$|\psi_A^{true}\rangle$ → True wave function of Hamiltonian H

$$E_A^{true} = \frac{\langle \psi_A^{true} | H | \psi_A^{true} \rangle}{\langle \psi_A^{true} | \psi_A^{true} \rangle}$$

Just in case the wf is not normalized ↓

$|\psi_A\rangle$ → trial wave function

$$E_A^{true} \leq E_A = \frac{\langle \psi_A | H | \psi_A \rangle}{\langle \psi_A | \psi_A \rangle}$$

This means that by asking

$$\left[\delta \left(\frac{\langle \psi_A | H | \psi_A \rangle}{\langle \psi_A | \psi_A \rangle} \right) = 0 \right]$$

we will the best approximation to E_A^{true} that is possible with the trial wf:

$$\psi_A = \mathcal{A} \left(\prod_j \phi_j(\vec{r}_j) \right)$$

→ That's why we do it

We solve it by

Lagrange multipliers

[LAGRANGE MULTIPLIERS:]

Minimize $\langle \psi_A | H | \psi_A \rangle$

w/ condition $\langle \psi_A | \psi_A \rangle = 1$

PROBLEM → min of $f(x)$ / $g(x) = 0$

SOLUTION →

Define $\mathcal{L}(x, \lambda) = f(x) - \lambda g(x)$

and minimize $\mathcal{L}(x, \lambda)$

instead

⇒ This will make our life much more simple

For Hartree-Fock :

$$\mathcal{L}(\phi_i, \lambda_i) = \langle \psi_A | H | \psi_A \rangle - \sum \lambda_i [\langle \phi_i | \phi_i \rangle - 1]$$

which we minimize :

$$\frac{\delta \mathcal{L}}{\delta \phi_j^*} \left[\langle \psi_A | H | \psi_A \rangle - \sum \lambda_i \langle \phi_i | \phi_i \rangle \right] = 0$$

notice that we can drop the "-1" above ($\frac{\delta}{\delta \phi_j^*}(-1) = 0$)

$$\langle \psi_A | H | \psi_A \rangle = \sum_i \langle \phi_i | \Pi_i | \phi_i \rangle + \frac{1}{2} \sum_{ij} \left(\langle \phi_i \phi_j | V | \phi_i \phi_j \rangle - \langle \phi_i \phi_j | V | \phi_j \phi_i \rangle \right)$$

HARTREE — Fock — Fermions

After minimization :

$$T_i|\phi_i\rangle + \sum_j \int d^3\vec{r}_j |\phi_j(\vec{r}_j)|^2 V(\vec{r}-\vec{r}_j)\phi_i(\vec{r}) - \sum_j \int d^3\vec{r}_j \phi_j^*(\vec{r}_j)\phi_j(\vec{r})V(\vec{r}-\vec{r}_j)\phi_i(\vec{r}_j) = \lambda_i \phi_i(\vec{r})$$

$$\lambda_i = \epsilon_i$$

→ Derived the same result as before

→ But we know something new:

[This solves a variational calculation]

BOTTOM-LINE

→ Solving HF should give us a decent approximation

PROBLEM

→ Difficulty of HF is set by choice of $V(\vec{r}_i - \vec{r}_j)$

the initial two-body potential

Extremely convenient choice:

$$\left[V(\vec{r}-\vec{r}') = C\,\delta(\vec{r}-\vec{r}') \right]$$

→ contact-range potentials

↓

Why convenient?

↳ [Fock term becomes local]

$$V^{Fock}(\vec{r}) = \pm \sum_j V(\vec{r}-\vec{r}')\,\phi_j^*(\vec{r})\,\phi_j(\vec{r}')$$

$$= \pm C\,\delta(\vec{r}-\vec{r}') \sum_j |\phi_j(\vec{r})|^2$$

LOCAL

contact-potentials → Extreme simplification of HF equations

Example : one-level system

only Hartree-term

$$T\phi(\vec{r}) + \int d^3\vec{r}\,' |\phi(\vec{r}\,')|^2 V(\vec{r}-\vec{r}\,')\phi(\vec{r}) = \epsilon\phi(\vec{r})$$

$$-C|\phi(\vec{r})|^2 = -C\rho(\vec{r})$$

density

$$\left[-\frac{\nabla^2}{2m}\phi(\vec{r}) - C\rho(\vec{r})\phi(\vec{r}) = \epsilon\phi(\vec{r})\right]$$

Actually its a bit weird

because $V^{MF}(\vec{r}) = -c|\phi(\vec{r})|^2$

Mean-field potential proportional

to the wave-function

square

However, easy to solve numerically

$$\left[-\frac{1}{2m}\vec{\nabla}^2 \phi(\vec{r}) - c\,|\phi(\vec{r})|^2 \phi(\vec{r})\right]$$

$$= \epsilon\,\phi(\vec{r})$$

=D You can expect contact-range

interactions to be popular

TOY MODEL

A-bosons, only 1-level

$$\left[-\frac{\nabla^2}{2m}\phi(\vec{r}) + 2C(A-1)|\phi(\vec{r})|^2\phi(\vec{r})\right] = \epsilon\phi(\vec{r})$$

(this could work up to $\Delta = 4$ in nuclei -> spin, isospin)

1) fix C to the deteron

→ $B(^4He) \sim 12$ MeV

2) fix C to the triton

→ $B(^4He) \sim 17$ MeV

$B_{exp}(^4He) \sim 28$ MeV

Good for a super-dumb model

Previous toy model is a silly example

(but shows why contact-range

two-body potentials are

a good choice)

⇓

SKYRME INTERACTION

$$V^{2B}_{ij}(\vec{r}_1-\vec{r}_2) = t_0(1+x_0P_\sigma)\delta^{(3)}(\vec{r}_1-\vec{r}_2)$$

$$+\frac{1}{2}t_1\left[\delta^{(3)}(\vec{r}-\vec{r}')(-\nabla'^2)+(-\nabla^2)\delta^{(3)}(\vec{r}_1-\vec{r}_2)\right]$$

$$+t_2\overleftarrow{\nabla}\delta^{(3)}(\vec{r}_1-\vec{r}_2)\cdot\overrightarrow{\nabla}$$

$$+iW_0(\vec{\sigma}_1+\vec{\sigma}_2)\cdot\left[\overleftarrow{\nabla}\times\left(\delta^{(3)}(\vec{r}_1-\vec{r}_2)\overrightarrow{\nabla}\right)\right]$$

$$V_{3B} = t_3\,\delta^{(3)}(\vec{r}_1-\vec{r}_2)\,\delta^{(3)}(\vec{r}_2-\vec{r}_3)$$

→ $t_0, x_0, t_1, t_2, W_0, t_3$ parameters

→ $\underline{P}_\sigma = \frac{1}{2}(1 + \vec{\sigma}_1 \cdot \vec{\sigma}_2)$

⇒ ∃ several parametrizations

(Skyrme I, II, III etc. ∿240)

GOGNY FORCES

$$V(\vec{r}_1 - \vec{r}_2) = \sum_{j=1}^{2} e^{-\frac{(\vec{r}_1 - \vec{r}_2)^2}{\mu_j^2}} (W_j + B_j \underline{P}_\sigma \quad \text{①}$$

$$- H_j \underline{P}_\tau - M_j \underline{P}_\sigma \underline{P}_\tau)$$

② $+ t_3 (1 + x_0 \underline{P}_\sigma) \delta^{(3)}(\vec{r}_1 - \vec{r}_2) \left[\rho\left(\frac{\vec{r}_1 + \vec{r}_2}{2}\right)\right]^\alpha$

$+ i W_{LS} \overleftarrow{\nabla} \delta(\vec{r}_1 - \vec{r}_2) \wedge \vec{\nabla} \cdot (\vec{\sigma}_1 + \vec{\sigma}_2)$

① → finite-range

② → Skyrme-like

Nuclear Physics
Volume 9, Issue 4, 1958–1959, Pages 615-634

→ SKYRME INTERACTION

The effective nuclear potential

T.H.R. Skyrme

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Abstract

An empirical analysis is made of the mean effective internucleon potential required in the shell-model description of nuclei, allowing for the presence of many-body effects as suggested by current theory. A consistent description is found in which the effective two-body interaction acts almost entirely in even states, and the many-body effects are simulated by a repulsive three-body contact interaction. The strength of the two-body interaction is consistent with that expressed by the free scattering matrix of the two-nucleon system, and that of the three-body interaction with the 'rearrangement energy' calculated in the many-body theory.

GOGNY FORCE ←

Hartree-Fock-Bogolyubov calculations with the $D1$ effective interaction on spherical nuclei

J. Dechargé and D. Gogny
Phys. Rev. C **21**, 1568 – Published 1 April 1980

Article PDF Export Citation

ABSTRACT

A self-consistent approach allowing the introduction of pairing into a comprehensive study of the bulk as well as the structure properties of nuclei is presented. It is emphasized that the density-dependent effective force used in the calculations reported here does permit the extraction of the mean field and the pairing field in the framework of the Bogolyubov theory. First, a brief review of Hartree-Fock-Bogolyubov formalism with density-dependent interactions is presented. Then the derivation of the effective interaction is explained and some details concerning the nuclear matter properties are given. Finally, we report the studies on spherical nuclei with special reference to the pairing properties. In order to demonstrate the versatility of our approach a comprehensive study of various nuclear properties is given. In view of the abundance of results obtained with our approach we plan to report the results on the deformed nuclei in a future publication.

NUCLEAR STRUCTURE Density-dependent Hartree-Fock-Bogolyubov (DDHFB) approximation applied to the calculations of the structure of spherical nuclei: binding energies, pairing correlations, density distributions, magnetic form factors, and quasiparticle spectra.

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→ The important thing is
to grasp the general idea

→ of course, it is a complex
subject

NEXT LESSON:

A few non-standard nuclei