NUCLEAR PHYSICS 22

OBTAINING A MEAN-FIELD POTENTIAL

HARTREE-FOCK, SKYRME, GOGNY

→ 2 OF 3 EXERCISE SETS
(3rd WILL COME SOON)

MAIN METHOD TO EVALUATE YOU

→ UNLESS THE SCHOOL REQUIRES IT, THERE WILL BE NO EXAM
(IF REQUIRED, IT WOULD BE EASY: CHOOSE BETWEEN A SET OF QUESTION)

→ IT'S POSSIBLE TO HAVE EXTRA SESSIONS FOR EXERCISES

$\boxed{\text{RECAP}}$ SHELL-MODEL $\Rightarrow$ two issues

1) How do I find a good V_{MF}?
(V_{MF} $\rightarrow$ mean field potential)

1.a) Convenient potential (Oscillator basis)

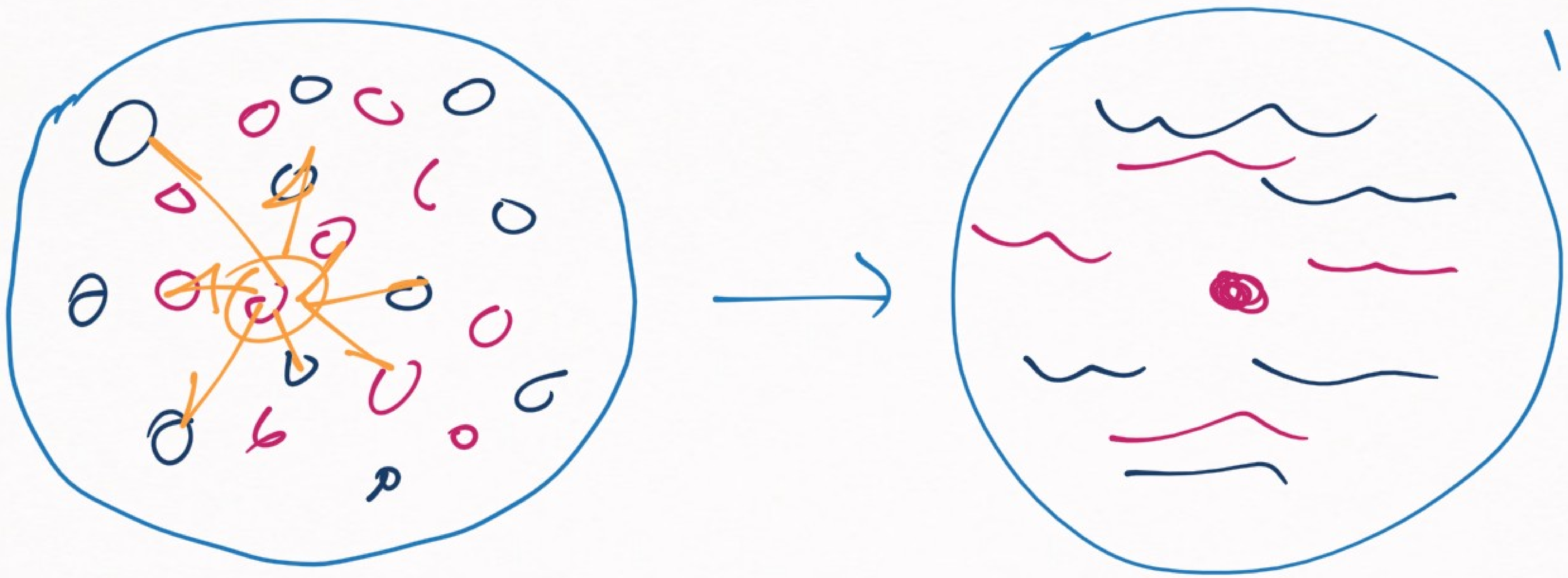
1.b) More theoretically-driven methods
(todays lesson)

2) How to deal w/ residual interactions?

→ last lesson (21)

MEAN FIELD POTENTIAL

Somehow we averge the individual interaction



[How to derive this average potential?]

God's view (we can calculate anything and know everything)

1) First, write the A-body Schrödinger eq.

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

Imagine → a) We know U_{ij}, etc.

b) We can solve it

2) With Ψ_A now we can get $\underline{\overline{V}_i}$ for each particle

avg V (a MF V)

$$\overline{V}_i(\vec{r}_i) = \sum_{j \neq i} \underbrace{\int \left(\prod_{j \neq i}\right) d^3\vec{r}_j}_{(A-1)\ d^3\vec{r}\ \text{integrals}} \left| \Psi_A(\ldots \vec{r}_i \ldots \vec{r}_j) \right|^2 V(\vec{r}_i - \vec{r}_j)$$

Alternatively, it can be written more elegantly

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

$$\overline{V}_i(\vec{r}) = \langle \Psi_n | \hat{V}_i(\vec{r}) | \Psi_n \rangle$$

(a second equivalent way to write the same thing)

3) Now, with $\bar{V}_i$, we can solve the monoparticular wave functions:

$$\left[-\frac{\nabla_i^2}{2m_i}+\bar{V}_i(\vec{r_i})\right]\phi_i(\vec{r})=\epsilon_i\phi(\vec{r})$$

4) Find the mean-field A-body wf:

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

FOR SIMPLICITY I WILL MOMENTARILY IGNORE ANTISYMMETRIZATION

1) + 2) + 3) + 4) → This assumes I know everything
(& I can calculate everything)

→ [MORE REALISTIC CHAIN OF
REASONING WILL BE :] ←

1) I have a two-body potential

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

but, I can't solve full Schrödinger

$$\left(\sum_i T_i + \sum_{ij} v_{ij}\right)\Psi_n = E_n \Psi_n$$ [CAN'T SOLVE]

2) I invent some one body potential

mean field

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

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

3) I will use the MF wave function to obtain a new MF potential

$$V_c^{(0)} \longrightarrow \Psi_A^{(0)} = \prod_i \phi_i^{(0)}(r_i)$$

$$V_i^{(1)} = \langle \Psi_A^{(0)} | \underbrace{\hat{V}_i(\vec{r})}_{\delta(\bar{r}-\bar{r}_i)\sum_{j\neq i} V(\vec{r}_i - \vec{r}_j)} | \Psi_A^{(0)} \rangle \longrightarrow \circledast$$

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

4) Repeat the process:

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

$$\longrightarrow \quad V_i^{(2)}(\vec{r})$$

5) Check for convergence :

$$\left.\begin{aligned} \phi_i^{(n+1)} &\simeq \phi_i^{(n)} \\ V_i^{(n+1)} &\simeq V_i^{(n)} \end{aligned}\right] \text{ITERATIVE PROCESS}$$

$\rightarrow$ [REALLY HARD WORK]

$[\phi^{(n+1)} = \phi^{(n)}] \rightarrow$ SELF-CONSISTENT CALCULATION

SO FAR, WE MADE A SIMPLIFICATION:

$\rightarrow$ Non-identical particles

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

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

→ WITH IDENTICAL PARTICLES:

nuclei

$$\Psi_0 = \mathcal{A}\left[\prod_j \phi_j(r_j)\right] \rightarrow \text{if fermions}$$

$$= \mathcal{S}\left[\prod_j \phi_j(r_j)\right] \rightarrow \text{if bosons}$$

↳ generate a nasty complication

[V mean-field will become non-local]

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

$$\pm \underbrace{\sum_{j \neq i} \int d^3\vec{r}_j \, \phi_j^*(\vec{r}_j) \, \phi_j(\vec{r}_i) \, V(\vec{r}_i - \vec{r}_j) \, \phi_i(\vec{r}_j)}_{\text{difficult (non-local) part}} \Big] = \epsilon_i \phi_i(\vec{r}_i)$$

+ for bosons

− for fermions

We got this type of non-local potential:

$$\left[-\frac{\nabla^2}{2m_i}\phi(\vec{r}) + \underbrace{\int d^3\vec{r}\,' \, v(\vec{r},\vec{r}\,')\,\phi(\vec{r}\,')}_{\text{this is the complication}}\right] = \epsilon\,\phi(\vec{r})$$

$$V(\vec{r},\vec{r}\,') = \Big[\delta^{(3)}(\vec{r}-\vec{r}\,')\sum_j \int d^3\vec{r}\,'' \,|\phi_j(\vec{r}\,'')|^2 \times v(\vec{r}-\vec{r}\,'')\Big] - \Big[\sum_j v(\vec{r}-\vec{r}\,')\,\phi_j^*(\vec{r}\,')\,\phi_j(\vec{r})\Big]$$

fermions

1 (LOCAL)

HARTREE TERM

2 (NON-LOCAL)

FOCK TERM

$\boxed{\text{RECAP}}$ → PREVIOUS FORMALISM

IS AIMED AT $\phi^{(n+1)} = \phi^{(n)}$

(SELF-CONSISTENT SOLUTION

THAT IS ATTAINED

BY MEANS OF ITERATION)

$$\begin{tikzcd} \phi^{(n)} \arrow[d] \\ {[\ldots]} \arrow[d] \\ \phi^{(n+1)} \arrow[uu, bend right] \end{tikzcd}$$

$\longrightarrow \exists$ a different way

[HARTREE-FOCK METHOD]

→ Simplify the previous calculation

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

→ actually not the full wavefunction

How to choose a good ψ_0?

VARIATIONAL PRINCIPLE :

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

$|\psi_A\rangle$ minimizes the energy of the system

$\boxed{|\psi_A^{true}\rangle}$ actually does this

$$|\psi_\Delta^{true}\rangle \longrightarrow E_\Delta^{true} = \frac{\langle \psi_\Delta^{true} | H | \psi_\Delta^{true} \rangle}{\langle \psi_\Delta^{true} | \psi_\Delta^{true} \rangle}$$

$|\psi_\Delta\rangle \longrightarrow$ "trial" wave function

$$E_\Delta^{true} \leq E_\Delta = \frac{\langle \psi_\Delta | H | \psi_\Delta \rangle}{\langle \psi_\Delta | \psi_\Delta \rangle}$$

However, we can try to minimize E_A w/ $\underbrace{\psi_A}_{\text{trial}}$

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

if this happens, we will get the best approximation to E_A^{true} w/ a family of trial wf's ψ_A

Trial wave function → $\Psi_A = \mathcal{A}\left(\prod_j \phi(r_j)\right)$

ASSUME A MEAN-FIELD TYPE OF SOLUTION

→ method of LAGRANGE MULTIPLIERS

REMINDER → $\boxed{\text{LAGRANGE MULTIPLIERS}}$

minimize $\langle \psi_\Delta | H | \psi_\Delta \rangle$ w/ condition $\langle \psi_\Delta | \psi_\Delta \rangle = 1$

$$\boxed{\min_{x} f(x) \;/\; g(x) = 0}$$

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

→ We minimize $\mathcal{L}(x,\lambda)$ in the usual way

(to make our lives easier)

$\boxed{\text{HF}}$ → $\mathcal{L}(\phi_i, \lambda_i) = \langle \phi_0 | H | \phi_0 \rangle$

$- \sum_i \lambda_i \left(\langle \phi_i | \phi_i \rangle - 1 \right)$

and we minimize ⟶

$$\rightarrow \frac{\delta}{\delta \phi_i^*}\left[\langle \psi_0 | H | \psi_0 \rangle - \sum_i{}' \lambda_i \langle \phi_i | \phi_i \rangle \right] = 0$$

I remove the "-1"
because $\frac{\delta}{\delta \phi_i^*}(-1) = 0$

$\mathcal{L} \rightarrow \phi_i^* \phi_i$

$\frac{\delta}{\delta \phi_i^*}$

$$\langle \Psi_A | H | \Psi_A \rangle = \sum_i \langle \phi_i | T_i | \phi_i \rangle + \frac{1}{2} \sum_{ij} \Big(\underbrace{\langle \phi_i \phi_j | V | \phi_i \phi_j \rangle}_{\text{HARTREE TERM}} \underbrace{-}_{\text{(Fermions)}} \underbrace{\langle \phi_i \phi_j | V | \phi_j \phi_i \rangle}_{\text{FOCK TERM}} \Big)$$

→ We still have to minimize :

$$T|\phi_i\rangle + \sum_j \int d^3\vec{r}_j \, |\phi_j(\vec{r}_i)|^2 \, V(\vec{r}_i-\vec{r}_j)\, \phi_i(\vec{r}_i)$$

$$- \sum_j \int d^3 \vec{r}_j \, \phi_j^*(r_j)\, \phi_j(\vec{r}_i)\, V(\vec{r}_i-\vec{r}_j)\, \phi_i(r_j)$$

$$= \lambda_i \, \phi_i(\vec{r}_i)$$

$$\lambda_i = \epsilon_i$$

→ this process led us to same result as before

→ but now it is formulated as solution of a variational problem

We only have to solve this w/ given $V(\vec{r}_i - \vec{r}_j)$ to obtain a decent approximation

$\boxed{\text{PROBLEM}}$ $\rightarrow$ Difficulty is set by our choice of $\underbrace{V(\vec{r}_i - \vec{r}_j)}$

initial two-body potential

[EXTREMELY CONVENIENT CHOICE]

$$\boxed{V(\vec{r}-\vec{r}') = C\,\delta(\vec{r}-\vec{r}')}$$

$\rightarrow$ contact-range potential ↳

Why is it convenient? $\rightarrow$ [FOCK TERM BECOMES LOCAL]

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

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

CONTACT-RANGE V $\Rightarrow$ LOCAL FOCK TERM

CALCULATION BECOME EASIER

Contact interactions → Extreme simplifications in HF equations

$\boxed{\text{EXAMPLE}}$ → one-level system $\phi_i \; (i=1)$

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

$$= \epsilon\phi(\vec{r}) \qquad |\phi(\vec{r})|^2 = \rho(\vec{r})$$

contact

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

→ density-dependent effective potentials

$\boxed{\text{TOY-MODEL}}$ → A-bosons, only 1-level

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

→ It can work up to A=4 (^4He) for nuclei.

1) fixed C to reproduce the deuteron

$\rightarrow B({}^4He) \sim 12\,MeV$

2) fixed C to reproduce Triton (${}^3He$)

$\rightarrow B({}^4He) \sim 17\,MeV$

$B_{exp}({}^4He) \sim 20\,MeV$

Really good for such a simple toy model

→ [tIF work better w/ contacts]

→ Historically, people have worked a lot w/ these contact-range potential models two important contact potential models:

1) SKYRME INTERACTION

2) GOGNY POTENTIAL

(not purely contact)

$\boxed{\text{SKYRME INTERACTION}}$

$$V_{2B}(\vec{r}_1 - \vec{r}_2) = t_0 (1 + x_0 P_\sigma)\, \delta^{(3)}(\vec{r}_1 - \vec{r}_2)$$

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

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

$$+ i W_0 (\vec{\sigma}_1 + \vec{\sigma}_2) \cdot \left[\vec{\nabla} \wedge \left(\delta^{(3)}(\vec{r}_1 - \vec{r}_2)\, \vec{\nabla} \right) \right]$$

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

→ $(x_0, t_0, t_1, t_2, w_0, t_3)$ → parameters

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

→ contacts wo/derivatives, w/ derivatives

D-wave, $\vec{L}\cdot\vec{S}$ term, 3-body contact

⇒ ∃ a lot of parametrization

(~ 240)

GOGNY FORCES

$$V(\bar{r}_1, \bar{r}_2) = \sum_{j=1}^{2} e^{-\frac{(\bar{r}_1-\bar{r}_2)^2}{\mu_j^2}} \left(W_j + B_j P_\sigma - H_j P_\tau - M_j P_\sigma P_\tau\right) \quad 1$$

$$+\, t_3 (1 + x_0 P_\sigma)\, \delta^{(3)}(\bar{r}_1 - \bar{r}_2) \left[\rho\left(\frac{\bar{r}_1+\bar{r}_2}{2}\right)\right]^{\alpha} + i W_{LS}\, \bar{\nabla}\, \delta(\bar{r}_1-\bar{r}_2) \wedge \bar{\nabla} \cdot (\bar{\sigma}_1 + \bar{\sigma}_2) \quad 2$$

① → finite-range

② → Skyrme-like

→ wonderful description of a lot of nuclei

$\geq$

ELSEVIER

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

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.

Skyrme

Gogny

18:45 39%

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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

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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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RECAP

→ Try to understand the general idea

→ this is a very complex subject, requires complicated calculations

(this is only for people doing this type of calculations)

→ Try not to do the exercises in the last moment