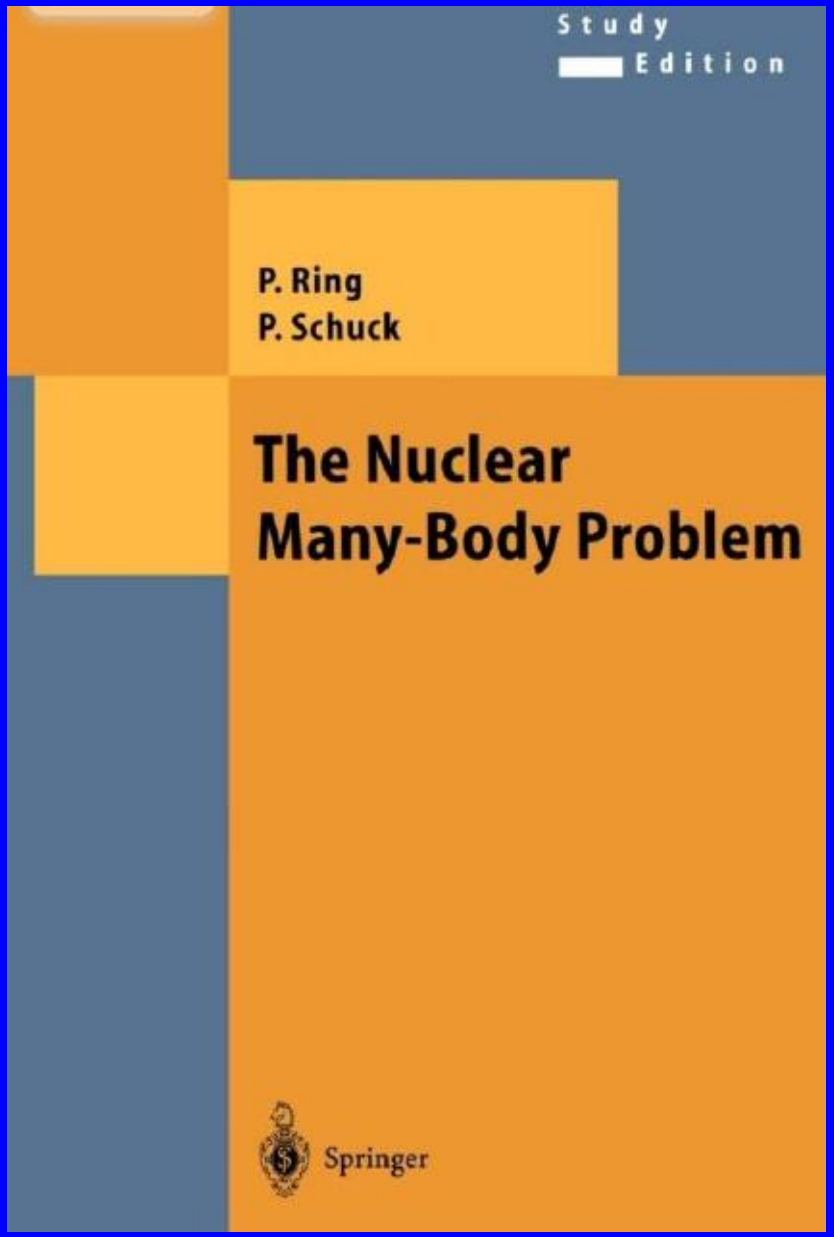
The International School "Nuclear Dynamics: from Stars to Colliders", JINR, June 29 –July 10, 2026.

Energy density functional and mean-field approach

Alexey P. Severyukhin

Bogoliubov Laboratory of Theoretical Physics
JINR

Reference


Study
Edition
P. Ring
P. Schuck
The Nuclear
Many-Body Problem
Springer

Lecture content

- The shell model approach to the many-body problem ➡
- The general variational principle ➡
- The Hartree-Fock method ➡
- The Hartree-Fock method in the Lipkin model ➡
- The structure of the nucleon-nucleon interaction ➡
- The Skyrme energy density functional (EDF) and the Hartree-Fock equations ➡
- Applications of Skyrme EDF to nuclear spectroscopy ➡

The shell model approach to the many-body problem

The single-particle model takes into account the individual nucleons. It provides a microscopic description of the nucleus. This is only an approximation of the exact many-body problem. However, the shell model can be used as a basis for many-body theories. First of all we discuss some general properites of the single particle model.

The microscopic theory of the nucleus is usually based on the following three properties.

- ✓ The nucleus is a quantum mechanical many-body system.
- ✓ The velocities in the nucleus are small enough so that one can neglect relativistic effects.
- ✓ The interaction between the nucleons has a two-body character.

The shell model approach to the many-body problem

A full microscopic theory of the nucleus would then be given by the solution of the many-body Schrödinger equation

$$H\Psi = \left\{ \sum_{i=1}^{A} -\frac{\hbar^2}{2m}\Delta_i + \sum_{i<j}^{A} v(i,j) \right\} \Psi(1,\ldots,A) = E\Psi(1,\ldots,A)$$

$i=\{r_i, s_i, t_i\}$ represents all coordinates of the ith nucleon, t is the isospin 1/2 for neutrons and – 1/2 for protons. With the assumption of the nuclear shell model, the above equation reduces to the much simpler equation

$$H_0\Psi = \left\{ \sum_{i=1}^{A} h_i \right\} \Psi = \sum_{i=1}^{A} \left\{ -\frac{\hbar^2}{2m}\Delta_i + V(i) \right\} \Psi = E\Psi$$

The wave functions are antisymmetrized products of single-particle functions.

The shell model approach to the many-body problem

The single- particle wavefunctions are eigenfunctions to the single-particle Hamiltonian

$$h_i\phi_k(i)=\epsilon_k\phi_k(i)$$

The single- particle wavefunctions provide an orthogonal basis for an occupation number representation within the second quantization. The level k corresponds a pair of creation and annihilation operators, which obey Fermi comutation relations. The shell model Hamiltonian has the following form

$$H_0=\sum\epsilon_k a_k^+ a_k$$

The eigen functions can be presented as

$$|\Phi_{k_1\ldots k_A}\rangle=a_{k_1}^+\ldots a_{k_A}^+|-\rangle$$

They are Slater determinants

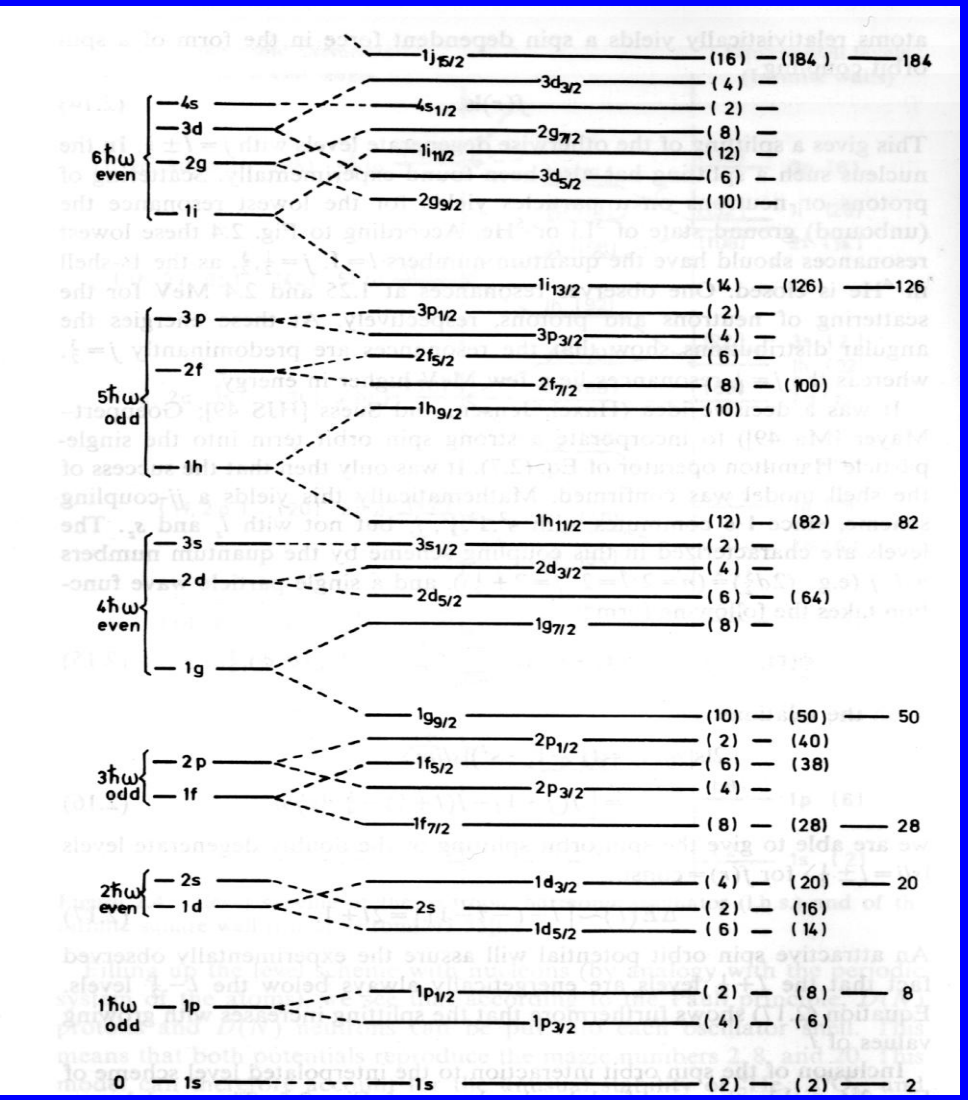
$$\Phi_{k_1\ldots k_A}(1,\ldots,A)=\begin{vmatrix}\phi_{k_1}(1) & \cdots & \phi_{k_1}(A)\\ \vdots & & \vdots\\ \phi_{k_A}(1) & & \phi_{k_A}(A)\end{vmatrix}$$

with eigenvales

$$E_{k_1\ldots k_A}=\epsilon_{k_1}+\cdots+\epsilon_{k_A}$$

The shell model approach to the many-body problem

Thus, we have for closed shells the following unique prescription for the construction of the A particle ground state as well as for the A particle excitation spectrum.



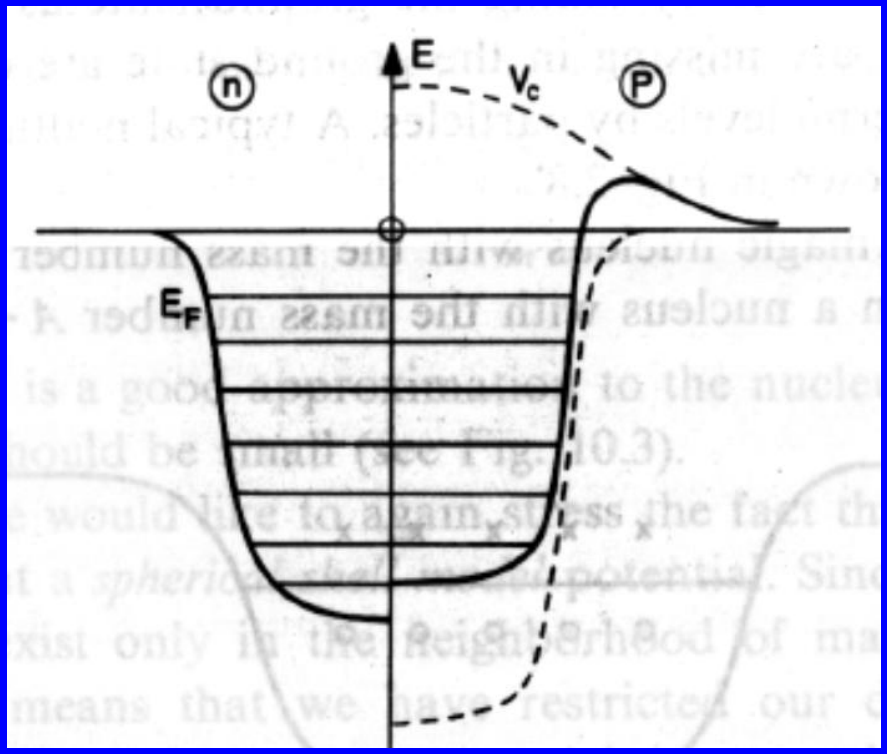
Starting with the $1s_{1/2}$ level, one has to occupy each level (nsljm) with just one particle until all A particles are used up. We obtain an A nucleon ground state where all different quantum states are occupied with just one particle up to the Fermi level (the highest occupied level); above the Fermi level all levels are unoccupied. The independent particle picture of the nucleus is different from that in an atom in the sense that in a nucleus there are two different kinds of particles, the proton and the neutron, whereas in an atom there is only the electron.

The shell model approach to the many-body problem

Protons and neutrons feel different mean-field potentials for two reasons.

$$V_C(\mathbf{r}) = \begin{cases} \frac{Ze^2}{R}\frac{1}{2}\left(3-\left(\frac{r}{R}\right)^2\right) & r \leqslant R \\ \frac{Ze^2}{r} & r > R \end{cases}$$

- ✓ Protons also interact via the Coulomb force. One usually adds the potential of a homogeneously charged sphere.
- ✓ The symmetry energy favors a configuration with an equal number of protons and neutrons. Because of the Coulomb repulsion for heavier nuclei, one has a neutron excess. The nuclear part of the proton potential is therefore deeper (see dashed line).



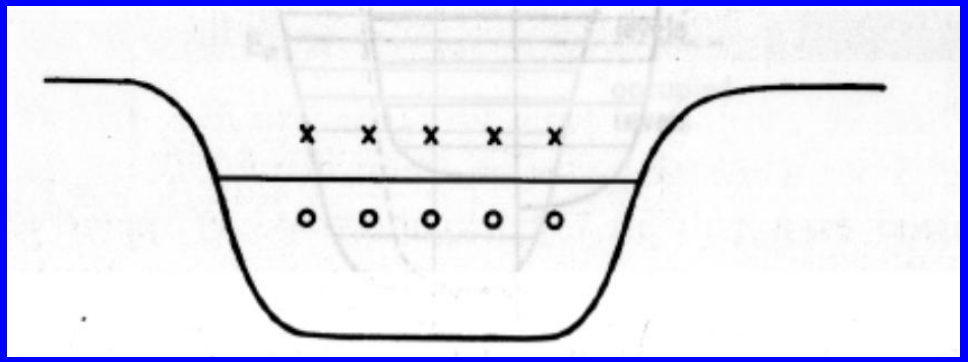
These two effects go in opposite directions, but they do not cancel.

The shell model approach to the many-body problem

The transfer of nucleons from below the Fermi level to levels above it.

$$|\Phi_{mi}\rangle := a_m^+ a_i |\Phi_0\rangle = \pm a_m^+ a_1^+ \ldots a_{i-1}^+ a_{i+1}^+ \ldots a_A^+ |-\rangle$$

$$\epsilon_{mi} = \epsilon_m - \epsilon_i$$



If we use the indices i, j for the levels below the Fermi surface, and the indices m , for the levels above the Fermi surface, the excitations in the shell model are then particle-hole excitations.

The multiparticle-multihole configuration is shown.

The Slater determinants form a complete set of states for the A nucleon system. Each state of the system is characterized by the distribution of the nucleons among the levels of the single particle potential, that is, by the "occupation numbers" of the levels. It is to classify all excited states by taking the ground state as a reference state.

The success of the phenomenologically introduced shell model justifies the assumption that nucleons move independently in an average potential produced by all of the nucleons. The question now is how to extract such a single-particle potential out of the sum of two-body interactions.

The general variational principle

We first want to show that the exact Schrödinger equation

$$H|\Psi\rangle = E|\Psi\rangle$$

is equivalent to the variational equation.

$$\delta E[\Psi] = 0,$$

$$E[\Psi] = \frac{\langle\Psi|H|\Psi\rangle}{\langle\Psi|\Psi\rangle}$$

The approximation of variational methods consists of the fact that |Ψ> is usually restricted to a set of mathematically simple trial wavefunctions. As soon as the true function is not in this set, the minimal solution is no longer the exact eigenfunction, but only an approximation. For any trial wavefunctions we can show

$$E[\Psi] \geq E_0$$

The general variational principle

To prove this, we develop the trial wave function in terms of the exact eigenfunctions of the Hamiltonian:

$$|\Psi\rangle = \sum_{n=0}^{\infty} a_n |\Psi_n\rangle$$

with

$$H|\Psi_n\rangle = E_n|\Psi_n\rangle$$

We obtain

$$E[\Psi] = \frac{\sum_{nn'} a_n^* a_n E_n \delta_{nn'}}{\sum_n |a_n|^2} \geqslant \frac{\sum_n |a_n|^2 E_0}{\sum_n |a_n|^2} = E_0$$

which is precisely

$$E[\Psi] \geqslant E_0$$

To find $|\Psi_1\rangle$, we must carry out the variation with the subsidiary condition

$$\langle \Psi_1 | \Psi_0 \rangle = 0$$

In principle we can continue and calculate the whole spectrum using this method.

The general variational principle

However, we do not know $|\Psi_0\rangle$ exactly. We find only an approximation $|\Phi_0\rangle$. For the calculation of an approximation $|\Phi_1\rangle$ to the first excited state $|\Psi_1\rangle$, we have to solve the variational equation $\delta E[\Psi]=0,$ with the supplementary condition that $|\Phi_1\rangle$ is orthogonal to $|\Phi_0\rangle$: $\langle\Phi_1|\Phi_0\rangle=0$ For the second excited state, we must have two supplementary conditions, $\langle\Phi_2|\Phi_1\rangle=0;$ and $\langle\Phi_2|\Phi_0\rangle=0$

The supplementary conditions are introduced via the Lagrange parameters. We can see that for higher excited states this method quickly gets rather complicated.We have shown that for a trial wave function, the ground state energy is always larger than or equal to the exact ground state energy and corresponds to an extremum. In order to decide which of two sets of trial wave functions is the better one, we have two criteria:

- ✓ If one set of the trial wave functions is a subset of the other, the larger set is usually the better one, because it contains the first's set minimum.
- ✓ Since the exact E is a lower bound, we may hope that out of two trial wave functions, the one for which the corresponding energy is closest to E is better.

Both criteria are not exact statements.

The Hartree-Fock method

Using the fact that the shell model has provided a suitable approximation for the qualitative explanation of many nuclear properties, we shall assume that there is an average single-particle potential (the Hartree-Fock potential) $H^{HF} = \sum_{i=1}^{A} h(i)$

whose eigenfunction having the lowest eigenvalue E_0 is an approximation to the exact ground state function. This eigenfunction $\Phi(1\ldots A)$ is a Slater determinant

$$|HF\rangle = |\Phi(1\ldots A)\rangle = \prod_{i=1}^{A} a_i^+ |-\rangle$$

in which the Fermion operators (a_k^+, a_k) correspond to the single-particle wave functions φ_k which are eigenfunctions of the single-particle Hamiltonian h,

$$h(i)\varphi_k(i) = \epsilon_k \varphi_k(i), \qquad i = \{\mathbf{r}_i, s_i, t_i\}$$

We can work in a configuration space based on some arbitrary complete and orthogonal set of single-particle wave functions $\{\chi_l\}$(an example is the set of spherical harmonic oscillator wave functions). $\varphi_k = \sum_l D_{lk}\chi_l$

The Hartree-Fock method

For each wave function χ_l, we define (c_l^+, c_l) and we can express $a_k^+ = \sum_l D_{lk} c_l^+$

Since both sets $\{\varphi_k\}$ and $\{\chi_l\}$ are complete and orthogonal, the transformation D has to be unitary:

$$D^+ D = D D^+ = 1$$

This fact also guarantees that (a_k^+, a_k) and (c_l^+, c_l) obey separate Fermi commutation relations. It is convenient to represent a Slater determinant $|\Phi\rangle$ by the single-particle density matrix $\rho_{ll'} = \langle \Phi | c_{l'}^+ c_l | \Phi \rangle$

$$\rho_{ll'} = \sum_{kk'} D_{lk} D_{l'k'}^* \langle \Phi | a_{k'}^+ a_k | \Phi \rangle = \sum_{i=1}^{A} D_{li} D_{l'i}^*$$

We carry out the variation which allows us to determine the HF-wave function $|\Phi\rangle$

We have to calculate the HF-energy $E^{HF} = \langle \Phi | H | \Phi \rangle$

The Hartree-Fock method

We start with the many-body Hamiltonian H and represent it in second quantization (c_l^+, c_l)

$$H = \sum_{l_1 l_2} t_{l_1 l_2} c_{l_1}^+ c_{l_2} + \frac{1}{4} \sum_{l_1 l_2 l_3 l_4} \bar{v}_{l_1 l_2, l_3 l_4} c_{l_1}^+ c_{l_2}^+ c_{l_4} c_{l_3}$$

$$\bar{v}_{l_1 l_2, l_3 l_4} = v_{l_1 l_2 l_3 l_4} - v_{l_1 l_2 l_4 l_3}.$$

Wick's theorem allows us to calculate the energy

$$E^{\mathrm{HF}} = \langle \Phi | H | \Phi \rangle$$

as a functional of the single-particle density

$$E^{\mathrm{HF}}[\rho] = \sum_{l_1 l_2} t_{l_1 l_2} \langle \Phi | c_{l_1}^+ c_{l_2} | \Phi \rangle + \frac{1}{4} \sum_{l_1 l_2 l_3 l_4} \bar{v}_{l_1 l_2 l_3 l_4} \langle \Phi | c_{l_1}^+ c_{l_2}^+ c_{l_4} c_{l_3} | \Phi \rangle$$

$$= \sum_{l_1 l_2} t_{l_1 l_2} \rho_{l_2 l_1} + \frac{1}{2} \sum_{l_1 l_2 l_3 l_4} \rho_{l_3 l_1} \bar{v}_{l_1 l_2 l_3 l_4} \rho_{l_4 l_2}$$

The Hartree-Fock method

To determine the HF-basis, we have to minimize the energy

$$E^{\mathrm{HF}} = \langle \Phi | H | \Phi \rangle$$

for all product wavefunctions . The variation of the energy is then given by

$$\delta E = E[\rho + \delta\rho] - E[\rho] = \sum_{kk'} h_{kk'} \delta\rho_{k'k} = \sum_{mi} h_{mi} \delta\rho_{im} + c.c.$$

where the Hermitian matrix h is defined as

$$h_{kk'} = \frac{\partial E^{\mathrm{HF}}[\rho]}{\partial \rho_{k'k}}$$

We obtain

$$h = t + \Gamma$$

with the self-consistent field

$$\Gamma_{kk'} = \sum_{ll'} \bar{v}_{kl'k'l} \rho_{ll'}$$

The Hartree-Fock method

Using eigenvalue problem we obtain the set of Hartree-Fock equations

$$\sum_{l'} h_{ll'} D_{l'k} = \sum_{l'} \left(t_{ll'} + \sum_{i=1}^{A} \sum_{pp'} \bar{v}_{lp'l'p} D_{pi} D^{*}_{p'i} \right) D_{l'k} = \epsilon_k D_{lk}$$

This is a nonlinear equation, and not easy to solve problem. The coefficients D are found by the solution of these equations. They determine the single-particle wave functions

$$\varphi_k = \sum_l D_{lk} \chi_l$$

We have thus derived the single-particle Hamiltonian

$$H^{\mathrm{HF}} = \sum_{kk'} h_{kk'} a_k^{+} a_{k'} = \sum_{kk'} (t + \Gamma)_{kk'} a_k^{+} a_{k'}$$

$$= \sum_{kk'} \left(t_{kk'} + \sum_{j=1}^{A} \bar{v}_{kjk'j} \right) a_k^{+} a_{k'} = \sum_{k} \epsilon_k a_k^{+} a_k$$

The single-particle Hamiltonian contains the kinetic energy and the self-consistent field which averages over all two-body interactions.

The Hartree-Fock method

To give a better interpretation of the Hartree-Fock equations, we write it in the coordinate space. Assuming a local two-body potential which does not depend on spin or isospin we find that

$$-\frac{\hbar^2}{2m}\Delta\varphi_k(\mathbf{r})+\sum_{j=1}^{A}\int d\mathbf{r}'\, v(\mathbf{r},\mathbf{r}')\cdot\varphi_j^*(\mathbf{r}')\{\varphi_j(\mathbf{r}')\varphi_k(\mathbf{r})-\varphi_j(\mathbf{r})\varphi_k(\mathbf{r}')\}$$
$$=\epsilon_k\varphi_k(\mathbf{r}).$$

We define the local Hartree potential

$$\Gamma_H(\mathbf{r})=\int d\mathbf{r}'\, v(\mathbf{r},\mathbf{r}')\sum_{j=1}^{A}|\varphi_j(\mathbf{r}')|^2=\int d\mathbf{r}'\, v(\mathbf{r},\mathbf{r}')\rho(\mathbf{r}')$$

and the nonlocal or exchange Fock potential

$$\Gamma_{Ex}(\mathbf{r},\mathbf{r}')=-v(\mathbf{r},\mathbf{r}')\sum_{j=1}^{A}\varphi_j^*(\mathbf{r}')\varphi_j(\mathbf{r})$$

We obtain

$$\left\{-\frac{\hbar^2}{2m}\Delta+\Gamma_H(\mathbf{r})\right\}\varphi_k(\mathbf{r})+\int d\mathbf{r}'\,\Gamma_{Ex}(\mathbf{r},\mathbf{r}')\varphi_k(\mathbf{r}')=\epsilon_k\varphi_k(\mathbf{r})$$

The nonlocal Schrödinger equations can be solved by iteration. Realistic HF calculations are difficult numerical problems.

The Hartree-Fock method in the Lipkin model

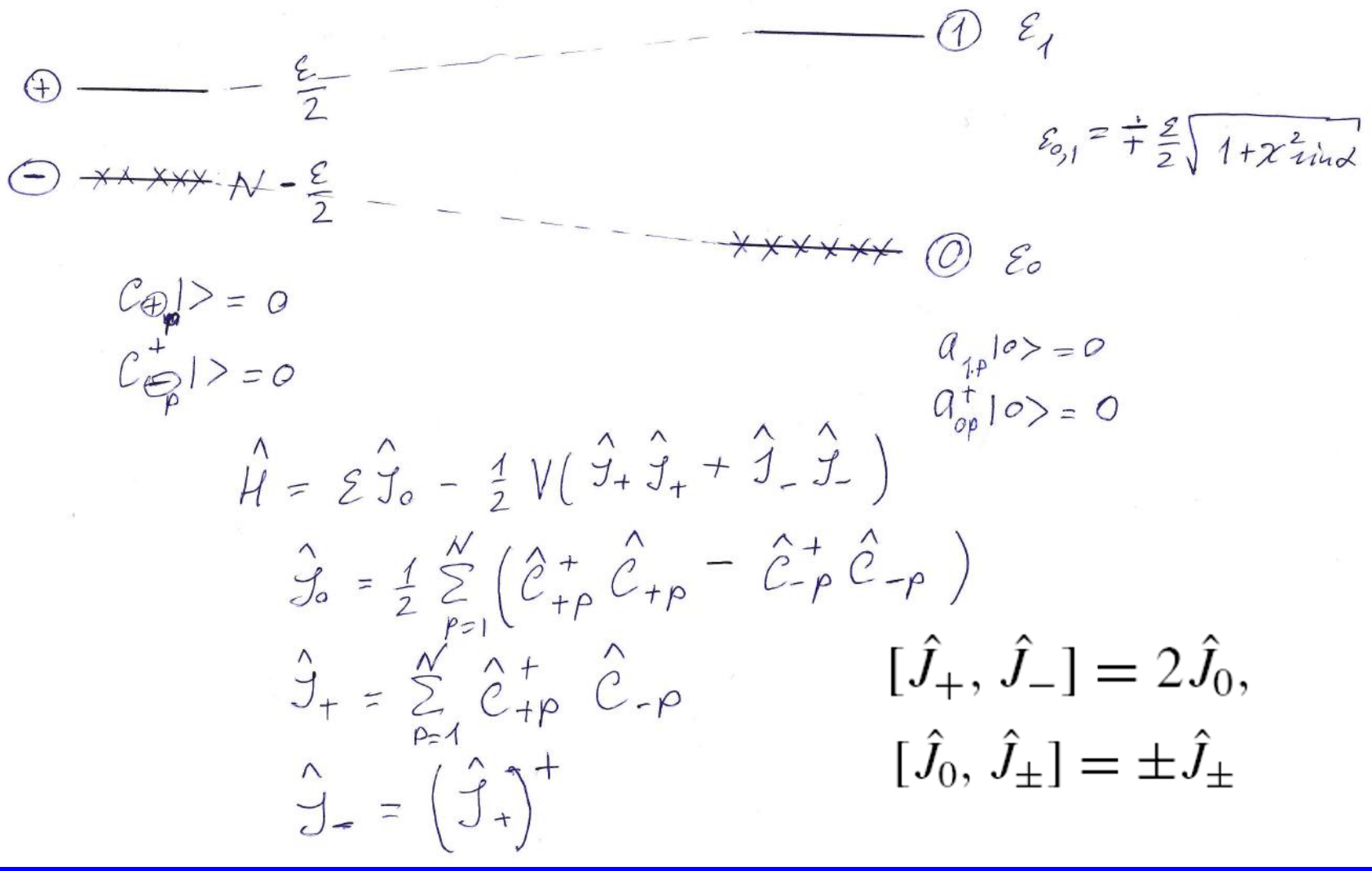
A. The model

Lipkin, Meshkov, and Glick introduced an exactly solvable model [8], usually called "Lipkin model" or "LMG model" in the literature, that has been widely used to test methods of approximation for the nuclear many-body problem.

The model consists of N fermions distributed in two N-fold degenerate shells separated by an energy ε. In their original paper, two different Hamiltonians were proposed. The one which is the most usually studied contains a monopole-monopole interaction and is given by

$$\hat{H} = \varepsilon \hat{J}_0 - \tfrac{1}{2} V (\hat{J}_+ \hat{J}_+ + \hat{J}_- \hat{J}_-), \qquad (1)$$

where V is the interaction strength and $\hat{J}_0$, $\hat{J}_\pm$ are quasispin operators [8–10]



The operators $\hat{c}^\dagger_{+p}$ and $\hat{c}^\dagger_{-p}$ create a particle in the upper or lower shells, respectively, where p labels the N degenerate levels within the shells. The operator $\hat{J}_0$ measures half of the difference between the number of particles in the upper and the lower levels.

B. Mean-field approximation

In mean-field, or Hartree-Fock (HF), approximation, the many-body wave function $|\alpha, \varphi\rangle$ is given by a Slater determinant

$$|\alpha, \varphi\rangle = \prod_{p=1}^{N} \hat{a}_{0p}^{\dagger} |-\rangle, \tag{4}$$

characterized by two real degrees of freedom α and φ, that will be specified below. The particle- and hole-creation operators of the corresponding HF single particle basis are given by a unitary transformation among the operators corresponding to the noninteracting basis [9,10]:

$$\begin{pmatrix} \hat{a}_{1p}^{\dagger} \\ \hat{a}_{0p}^{\dagger} \end{pmatrix} = \begin{pmatrix} \cos(\alpha) & -\sin(\alpha) e^{-i\varphi} \\ \sin(\alpha) e^{i\varphi} & \cos(\alpha) \end{pmatrix} \begin{pmatrix} \hat{c}_{+p}^{\dagger} \\ \hat{c}_{-p}^{\dagger} \end{pmatrix}. \tag{5}$$

The constrained HF ground-state energy is a function of the variables α and φ:

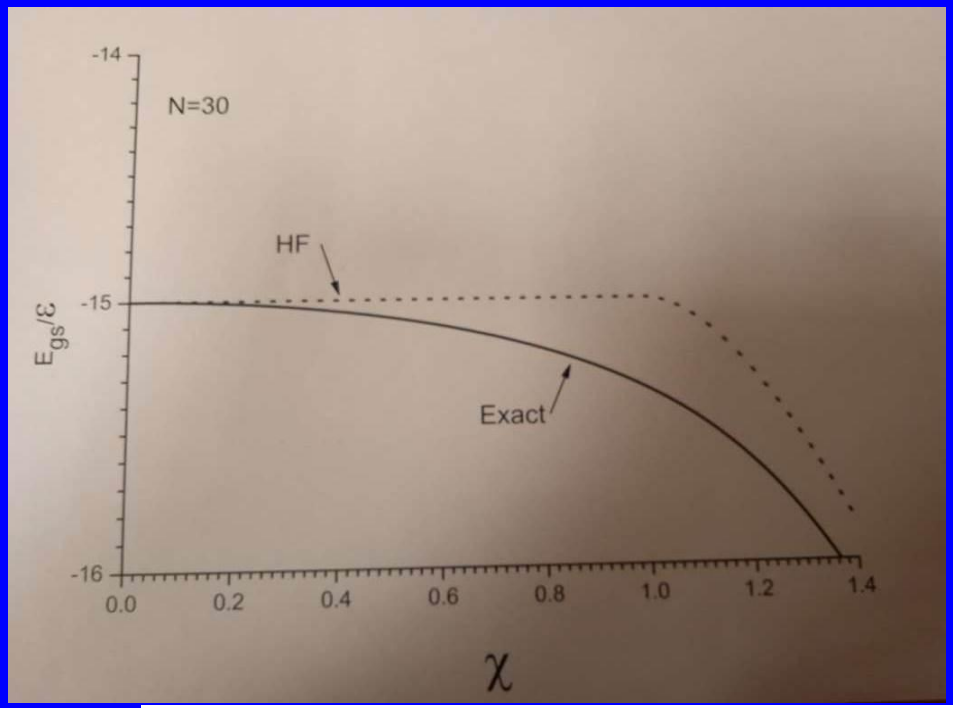
$$E_{gs}^{\mathrm{HF}}(\alpha, \varphi) = -\frac{\varepsilon N}{2}\left[\cos(2\alpha) + \frac{1}{2}\chi \sin^2(2\alpha)\cos(2\varphi)\right], \quad (7)$$

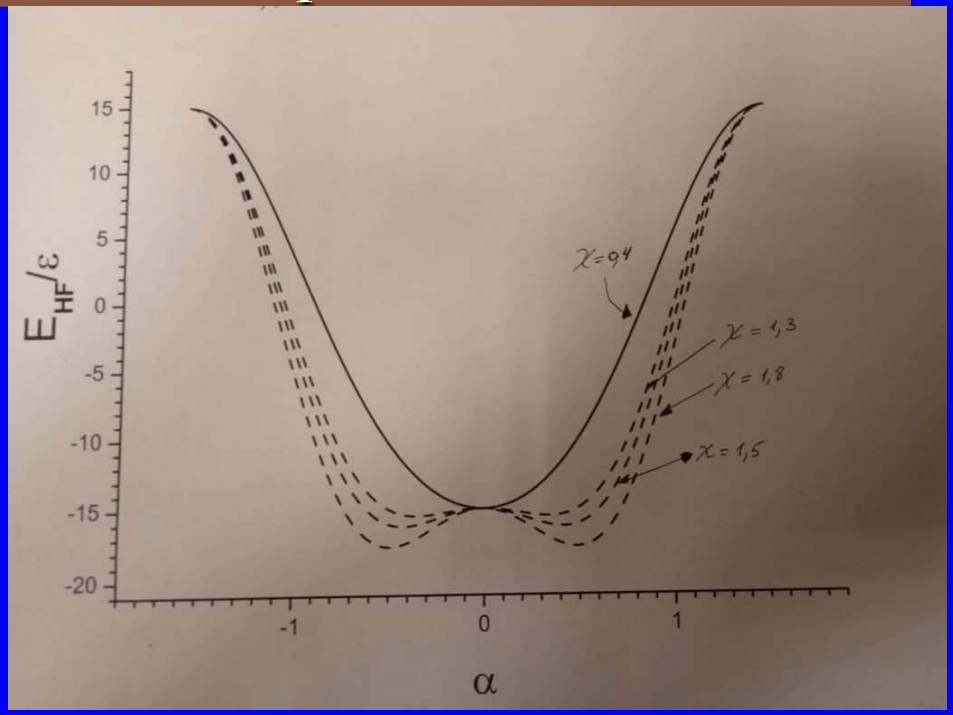
where

$$\chi = \frac{(N-1)\,V}{\varepsilon}. \quad (8)$$

Note that, for a given value of α, the lowest HF state always corresponds to $\varphi = 0$. The eigenvalues of the single-particle Hamiltonian, usually called single-particle energies, depend on α only for any mean-field state $|\alpha, \varphi\rangle$.

The Hartree-Fock method in the Lipkin model





One can identify the variable α as a deformation parameter. There is a phase transition at $\chi = 1$ from a spherical ($\alpha = \varphi = 0$) to a "deformed" ground state. In the latter case, the value of α is obtained by solving the equation $\chi \cos(2\alpha) = 1$. The phase transition and the properties of exact and approximated ground states in this regime were first discussed by Agassi *et al.* [15].

PHYSICAL REVIEW C **74**, 024311 (2006)

A. P. SEVERYUKHIN, M. BENDER, AND P.-H. HEENEN

Lipkin model on a quantum computer

Michael J. Cervia,[1,*] A. B. Balantekin,[1,†] S. N. Coppersmith,[1,2,‡] Calvin W. Johnson,[3,§] Peter J. Love,[4,5,‖] C. Poole,[1,¶] K. Robbins,[4,**] and M. Saffman[1,††]

[1]*Department of Physics, University of Wisconsin–Madison, Madison, Wisconsin 53706, USA*
[2]*School of Physics, The University of New South Wales, Sydney, New South Wales 2052, Australia*
[3]*Department of Physics, San Diego State University, San Diego, California 92182-1233, USA*
[4]*Department of Physics and Astronomy, Tufts University, Medford, Massachusetts 02155, USA*
[5]*Computational Science Initiative, Brookhaven National Laboratory, Upton, New York, 11973-5000, USA*

(Received 7 April 2021; accepted 7 July 2021; published 3 August 2021)

Atomic nuclei are important laboratories for exploring and testing new insights into the universe, such as experiments to directly detect dark matter or explore properties of neutrinos. The targets of interest are often heavy, complex nuclei that challenge our ability to reliably model them (as well as quantify the uncertainty of those models) with classical computers. Hence there is great interest in applying quantum computation to nuclear structure for these applications. As an early step in this direction, especially with regards to the uncertainties in the relevant quantum calculations, we develop circuits to implement variational quantum eigensolver (VQE) algorithms for the Lipkin-Meshkov-Glick model, which is often used in the nuclear physics community as a testbed for many-body methods. We present quantum circuits for VQE for two and three particles and discuss the construction of circuits for more particles. Implementing the VQE for a two-particle system on the IBM Quantum Experience, we identify initialization and two-qubit gates as the largest sources of error. We find that error mitigation procedures reduce the errors in the results significantly, but additional quantum hardware improvements are needed for quantum calculations to be sufficiently accurate to be competitive with the best current classical methods.

PHYSICAL REVIEW C **109**, 024327 (2024)

Solving the Lipkin model using quantum computers with two qubits only with a hybrid quantum-classical technique based on the generator coordinate method

Yann Beaujeault-Taudière *
Université Paris-Saclay, CNRS/IN2P3, IJCLab, 91405 Orsay, France
and Laboratoire Leprince-Ringuet (LLR), École Polytechnique, CNRS/IN2P3, F-91128 Palaiseau, France

Denis Lacroix †
Université Paris-Saclay, CNRS/IN2P3, IJCLab, 91405 Orsay, France

(Received 11 December 2023; accepted 31 January 2024; published 27 February 2024)

The possibility of using the generator coordinate method (GCM) using hybrid quantum-classical algorithms with reduced quantum resources is discussed. The task of preparing the basis states and calculating the various kernels involved in the GCM is assigned to the quantum computer, while the remaining tasks, such as finding the eigenvalues of a many-body problem, are delegated to classical computers for post-processing the generated kernels. This strategy reduces the quantum resources required to treat a quantum many-body problem. We apply the method to the Lipkin model. Using the permutation symmetry of the Hamiltonian, we show that, ultimately, only two qubits is enough to solve the problem regardless of the particle number. The classical computing post-processing leading to the full energy spectrum can be made using standard generalized eigenvalues techniques by diagonalizing the so-called Hill-Wheeler equation. As an alternative to this technique, we also explored how the quantum state deflation method can be adapted to the GCM problem. In this method, variational principles are iteratively designed to access the different excited states with increasing energies. The methodology proposed here is successfully applied to the Lipkin model with a minimal size of two qubits for the quantum register. The performances of the two classical post-processing approaches with respect to the statistical noise induced by the finite number of measurements and quantum devices noise are analyzed. Very satisfactory results for the full energy spectra are obtained once noise corrections techniques are employed.

The structure of the nucleon-nucleon interaction

We wish to apply the techniques of modern many-body theory. We also follow three basic assumptions:

- ✓ Dynamical mesonic degrees of freedom can be neglected and the nucleus can be described as a system of A nucleons whose interaction can be represented by a potential.
- ✓ Relativistic effects are negligible.
- ✓ Only two-body forces are important.

Even with these rather drastic assumptions, we immediately run into difficulties. There exists no derivation of the nucleon-nucleon force from first principles. This should be possible in principle with the modern theory of gauge fields for quarks and gluons. On the other hand, the bare nuclear forces are, from a numerical point of view, very ill behaved. They show strong repulsion at short distances (hard core) and cannot be treated straightforwardly by the usual many-body techniques. I will focus on the phenomenological effective forces, which are constructed on the basis of these considerations, but depend on some parameters that are adiusted to fit experimental data.

The structure of the nucleon-nucleon interaction

Let me remind general properties of a two-body force. The most general quantum mechanical two-body potential V is completely specified by its matrix elements between two-body states in the coordinate representation:

$$\langle \mathbf{r}_1' s_1' t_1' \mathbf{r}_2' s_2' t_2' | V | \mathbf{r}_1 s_1 t_1 \mathbf{r}_2 s_2 t_2 \rangle$$

We require the following eight symmetries:

1. Hermitianity.
2. Invariance under an exchange of the coordinates. This property is strongly connected with the symmetry of the two-particle wave function |12>. Since nucleons are fermions, they have to be totally antisymmetric.

$$V(1,2) = V(2,1)$$

$$\langle \mathbf{r}_1 s_1 t_1, \mathbf{r}_2 s_2 t_2 \mid 12 \rangle = \varphi(\mathbf{r}_1, \mathbf{r}_2)\chi(s_1, s_2)\zeta(t_1, t_2)$$

φ	χ	abbreviation	ζ
even	singlet	es	+
even	triplet	et	−
odd	singlet	os	−
odd	triplet	ot	+

The structure of the nucleon-nucleon interaction

3. Translational invariance. The potential depends on the relative coordinate $\mathbf{r} = \mathbf{r}_1 - \mathbf{r}_2$

$$V(1,2) = V(\mathbf{r}, \mathbf{p}_1, \boldsymbol{\sigma}^{(1)}, \boldsymbol{\tau}^{(1)}, \mathbf{p}_2, \boldsymbol{\sigma}^{(2)}, \boldsymbol{\tau}^{(2)}).$$

4. Galilean invariance. The potential is not changed by a transformation to a system which moves with constant velocity, that is, it depends only on the relative momentum $\mathbf{p} = \frac{1}{2}(\mathbf{p}_1 - \mathbf{p}_2)$

$$V(1,2) = V(\mathbf{r}, \mathbf{p}, \boldsymbol{\sigma}^{(1)}, \boldsymbol{\tau}^{(1)}, \boldsymbol{\sigma}^{(2)}, \boldsymbol{\tau}^{(2)})$$

5. Invariance under space reflection. Contrary to the weak interaction, there is no parity violation for strong interactions.

$$V(\mathbf{r}, \mathbf{p}, \boldsymbol{\sigma}^{(1)}, \boldsymbol{\tau}^{(1)}, \boldsymbol{\sigma}^{(2)}, \boldsymbol{\tau}^{(2)}) = V(-\mathbf{r}, -\mathbf{p}, \boldsymbol{\sigma}^{(1)}, \boldsymbol{\tau}^{(1)}, \boldsymbol{\sigma}^{(2)}, \boldsymbol{\tau}^{(2)})$$

6. Time reversal invariance guarantees that the equations of motion do not depend on the direction in which the time evolves

$$V(\mathbf{r}, \mathbf{p}, \boldsymbol{\sigma}^{(1)}, \boldsymbol{\tau}^{(1)}, \boldsymbol{\sigma}^{(2)}, \boldsymbol{\tau}^{(2)}) = V(\mathbf{r}, -\mathbf{p}, -\boldsymbol{\sigma}^{(1)}, \boldsymbol{\tau}^{(1)}, -\boldsymbol{\sigma}^{(2)}, \boldsymbol{\tau}^{(2)})$$

The structure of the nucleon-nucleon interaction

7. Rotational invariance in coordinate space. Rotations in three-dimensional coordinate space act not only on the vectors r and p but also on the spin matrices. It has to be a scalar under a rotation in coordinate space, which means that V has to be a scalar. There exist three independent scalars which we can construct from the two vectors $\mathbf{r}$ and $\mathbf{p}$, namely $\mathbf{r}^2$, $\mathbf{p}^2$ $\boldsymbol{rp}+\boldsymbol{pr}$. However, $\boldsymbol{rp}+\boldsymbol{pr}$ can only appear quadratically because of time reversal invariance. It is more convenient to express $(\boldsymbol{rp}+\boldsymbol{pr})^2$ through $\mathbf{r}^2$, $\mathbf{p}^2$ and $\boldsymbol{L}^2=(\boldsymbol{r}\times\boldsymbol{p})^2$. Before we find that $V(\mathbf{r},\mathbf{p},\boldsymbol{\sigma}^{(1)},\boldsymbol{\sigma}^{(2)})=V(\mathbf{r},\mathbf{p},\boldsymbol{\sigma}^{(2)},\boldsymbol{\sigma}^{(1)})$

The possible independent combinations $\boldsymbol{\sigma}^{(1)}\boldsymbol{\sigma}^{(2)}$, $(\mathbf{r}\boldsymbol{\sigma}^{(1)})(\mathbf{r}\boldsymbol{\sigma}^{(2)})$, $(\mathbf{p}\boldsymbol{\sigma}^{(1)})(\mathbf{p}\boldsymbol{\sigma}^{(2)})$, $(\mathbf{L}\boldsymbol{\sigma}^{(1)})(\mathbf{L}\boldsymbol{\sigma}^{(2)})+(\mathbf{L}\boldsymbol{\sigma}^{(2)})(\mathbf{L}\boldsymbol{\sigma}^{(1)})$.

Each of these terms can be multiplied by an arbitrary function of $\mathbf{r}^2$, $\mathbf{p}^2$ and $\boldsymbol{L}^2$

8. Rotational invariance in isospin space. Within the isospin formalism, protons and neutrons are considered as quantum states of one elementary particle that form a doublet with isospin 1/2. The presentation of the rotational group reproduces all properties.

$V_0+V_\tau\boldsymbol{\tau}^{(1)}\boldsymbol{\tau}^{(2)}$

The structure of the nucleon-nucleon interaction

(i). Among the local forces, which do not depend on the velocity, the *central force* is the most important. It depends only on the distance r between the nucleons:

$$V_C(1,2) = V_0(r) + V_\sigma(r)\boldsymbol{\sigma}^{(1)}\boldsymbol{\sigma}^{(2)} + V_\tau(r)\boldsymbol{\tau}^{(1)}\boldsymbol{\tau}^{(2)} + V_{\sigma\tau}(r)\boldsymbol{\sigma}^{(1)}\boldsymbol{\sigma}^{(2)}\boldsymbol{\tau}^{(1)}\boldsymbol{\tau}^{(2)}.$$

(ii). The only remaining local part is the *Tensor force*

$$V_T(1,2) = \left[V_{T_0}(r) + V_{T_\tau}(r)\boldsymbol{\tau}^{(1)}\boldsymbol{\tau}^{(2)} \right] \cdot S_{12}$$

with

$$S_{12} = \frac{3}{r^2}(\boldsymbol{\sigma}^{(1)}\mathbf{r})(\boldsymbol{\sigma}^{(2)}\mathbf{r}) - \boldsymbol{\sigma}^{(1)}\boldsymbol{\sigma}^{(2)}.$$

The term $-\boldsymbol{\sigma}^{(1)}\boldsymbol{\sigma}^{(2)}$ is added to make sure that an average of $V_T(1,2)$ taken over all directions of $\mathbf{r}$ vanishes:

$$\int V_T(1,2)\, d\Omega = 0 \quad \text{where} \quad \mathbf{r} = (r, \Omega).$$

An experimental hint of the existence of a tensor component in the nucleon–nucleon potential is given by the quadrupole moment of the deuteron, which cannot be explained by pure central forces.

The structure of the nucleon-nucleon interaction

The central force can also be represented in terms of exchange or projection operators.

$$P^{\sigma}=\frac{1}{2}(1+\boldsymbol{\sigma}^{(1)}\boldsymbol{\sigma}^{(2)}), \qquad P^{\tau}=\frac{1}{2}(1+\boldsymbol{\tau}^{(1)}\boldsymbol{\tau}^{(2)})$$

We can apply P^{σ}

$$P^{\sigma}\varphi(\mathbf{r}_1\mathbf{r}_2)\chi(s_1,s_2)\zeta(t_1,t_2)=\varphi(\mathbf{r}_1,\mathbf{r}_2)\chi(s_2,s_1)\zeta(t_1,t_2)$$

This is easy to understand by using the operator of the total spin S. The eigenstates of S are singlet and triplet states

$$P^{\sigma}=\frac{1}{2}(1+2(\mathbf{S}^2-\mathbf{s}^{(1)^2}-\mathbf{s}^{(2)^2}))=S(S+1)-1=\begin{cases}1 & \text{for triplet}\\ -1 & \text{for singlet.}\end{cases}$$

The Pauli principle may be written in the following form $P^{r}P^{\sigma}P^{\tau}=-1$

We can express the operator $P^{\tau}=-P^{r}P^{\sigma}$ eliminate the products $\boldsymbol{\sigma}^{(1)}\boldsymbol{\sigma}^{(2)}$ $\boldsymbol{\tau}^{(1)}\boldsymbol{\tau}^{(2)}$

Therefore we obtain the central force

$$V_C=V_{\mathrm{W}}(r)+V_{\mathrm{M}}(r)P^{r}+V_{\mathrm{B}}(r)P^{\sigma}+V_{\mathrm{H}}(r)P^{r}P^{\sigma}$$

V_{W} (Wigner force)
V_{M} (Majorana force)
V_{B} (Bartlett force)
V_{H} (Heisenberg force)

The structure of the nucleon-nucleon interaction

I turn out to the phenomenological effective interactions between nucleons. We face a certain number of fit parameters adjusted to reproduce the experimental data. In many cases this procedure has turned out to be extremely successful and the experimental data covering quite a large range of nuclear masses can be explained. There exists, of course, an enormous number of different phenomenological interactions that have been applied to problems in nuclear physics. Each of them has been used for a specific problem and their range of validity and success very much. During my lecture I cannot give a complete picture, and I will restrict our discussion to the most successful examples. We prefer to choose the analytical form of the effective interaction to be as simple as possible. For example, we assume that the effective interaction obeys the invariance principles. We know that the range of the nuclear force is rather short. The simplest ansatz therefore consists in using a zero range force whose radial dependence is described by δ-function. In fact, such forces turn out to be rather useful because they are simple to handle and they describe many nuclear properties quite well. More realistic forces, however, need to have a finite non-vanishing range.

The structure of the nucleon-nucleon interaction

The finite range can be simulated by a momentum dependence. To show this we transform a function V(r) of the relative distance $\boldsymbol{r} = \boldsymbol{r_1} - \boldsymbol{r_2}$ into momentum space

$$\langle \mathbf{p}|V|\mathbf{p}'\rangle = \frac{1}{(2\pi\hbar)^3}\int e^{-\frac{i}{\hbar}(\mathbf{p}-\mathbf{p}')\mathbf{r}} V(\mathbf{r}) d^3r$$

We see that a δ-force is a constant and that any range represents a p-dependence in momentum space. The simplest rotationally invariant one is of the following form

$$(2\pi\hbar)^3\langle \mathbf{p}|V|\mathbf{p}'\rangle = V_0 + V_1\mathbf{p}'^2 + V_1\mathbf{p}^2 + V_2\mathbf{p}\mathbf{p}'$$

which in coordinate space corresponds to the momentum dependent operator

$$V(\mathbf{r}) = V_0\delta(\mathbf{r}) + V_1(\hat{\mathbf{p}}^2\delta(\mathbf{r}) + \delta(\mathbf{r})\hat{\mathbf{p}}^2) + V_2\hat{\mathbf{p}}\delta(\mathbf{r})\hat{\mathbf{p}}$$

Effective forces usually depend on nucleon density. Such density dependence is easy to understand if , for example, we consider three-body term as an equivalent to a density dependent two-body force.

The structure of the nucleon-nucleon interaction

In 1956 T.H.R. Skyrme proposed an effective interaction:

$$V = \sum_{i<j} V(i,j) + \sum_{i<j<k} V(i,j,k)$$

To simplify the calculations, he used a short-range expansion for the two-body part:

$$\begin{aligned} V(1,2) = {} & t_0(1 + x_0 P^\sigma)\delta(\mathbf{r}_1 - \mathbf{r}_2) \\ & + \tfrac{1}{2} t_1 \left[\delta(\mathbf{r}_1 - \mathbf{r}_2)\mathbf{k}^2 + \mathbf{k}^2 \delta(\mathbf{r}_1 - \mathbf{r}_2) \right] + t_2 \mathbf{k} \delta(\mathbf{r}_1 - \mathbf{r}_2)\mathbf{k} \\ & + i W_0 (\boldsymbol{\sigma}^{(1)} + \boldsymbol{\sigma}^{(2)})\mathbf{k} \times \delta(\mathbf{r}_1 - \mathbf{r}_2)\mathbf{k}, \end{aligned}$$

where $\mathbf{k} = (1/\hbar)\mathbf{p}$ is the operator of the relative momentum $\mathbf{k} = \frac{1}{2i}(\nabla_1 - \nabla_2)$

For the three-body force Skyrme also assumed a zero range force

$$V(1,2,3) = t_3 \delta(\mathbf{r}_1 - \mathbf{r}_2)\delta(\mathbf{r}_2 - \mathbf{r}_3)$$

The parameters $t_0 t_1 t_2 t_3$ x_0 W_0 were adjusted to the experimental binding energies and radii. The parameters t_0 and x_0 describes a pure δ-force with a spin-exchange; $t_1 t_2$ simulate an effective range. The fourth term represents a two-body spin orbit interaction. The three-body term turns out to be equivalent to a density dependent two-body interaction:

$$V_\rho(1,2) = \frac{1}{6} t_3 (1 + P^\sigma)\delta(\mathbf{r}_1 - \mathbf{r}_2)\rho\left(\tfrac{1}{2}(\mathbf{r}_1 + \mathbf{r}_2)\right)$$

The structure of the nucleon-nucleon interaction

There are essentially three reasons why this force is so popular:

- ✓ In 1972 D. Vautherin and D. M. Brink were able to reproduce the nuclear binding energies over the whole periodic table with a reasonable set of parameters and, at the same time, the nuclear radii. This had not been possible with the usual non-density dependent forces.
- ✓ In 1972 J. W. Negele and D. Vautherin gave the connection between this force and the more fundamental G-matrix theory.
- ✓ The mathematical form of the force is extremely simple. The δ-functions simplify all types of calculations enormously.

The structure of the nucleon-nucleon interaction

The Gogny Interaction. Despite the great success of the Skyrme interaction, it has been argued that zero range forces might not be able to simulate the long range or even the intermediate range parts of the realistic effective interaction. In particular, the Skyrme force are not able to properly describe pairing correlations in nuclei. In 1975 D. Gogny replaced the $t_0 t_1 t_2$ parts of the Skyrme force by a sum of two of Gaussians with spin-isospin exchange mixtures

$$V(1,2) = \sum_{i=1}^{2} e^{-(\mathbf{r}_1-\mathbf{r}_2)^2/\mu_i^2}(W_i + B_i P^\sigma - H_i P^\tau - M_i P^\sigma P^\tau)$$
$$+ iW_0(\boldsymbol{\sigma}_1+\boldsymbol{\sigma}_2)\mathbf{k}\times\delta(\mathbf{r}_1-\mathbf{r}_2)\mathbf{k}$$
$$+ t_3(1+P^\sigma)\delta(\mathbf{r}_1-\mathbf{r}_2)\rho^{1/3}(\tfrac{1}{2}(\mathbf{r}_1+\mathbf{r}_2)).$$

The parameters were adjusted to the properties of finite nuclei, and for nuclear matter.

The structure of the nucleon-nucleon interaction

This force was proposed by A. B. Migdal in the theory of finite Fermi systems. Based on the interacting quasiparticle concept of Landau's theory of a Fermi liquid, A. B. Migdal introduces this force to describe the collective excitations in nuclei.

Starting from the ground state of an even-even system, the quasiparticles are defined as the low-lying excitations in the neighboring odd mass nuclei. The ground state of the even system contains no quasiparticles, and excited states are characterized by the quasiparticle occupation numbers n_λ. A change of the occupation numbers δn_λ leads to a change in the total energy

$$\delta E_0 = \sum_\lambda \epsilon_\lambda^0 \delta n_\lambda + \frac{1}{2} \sum_{\lambda\lambda'} F_{\lambda\lambda'} \delta n_\lambda \delta n_{\lambda'}$$

where ϵ_λ^0 are the energies of a quasiparticle λ in the absence of any other quasiparticle and $F_{\lambda'\lambda}$ is the so-called quasiparticle interaction. In an infinite system with translational invariance, the quasiparticles are characterized by the momentum **k.** Particle-hole interaction is given by

$$F^{ph}(\mathbf{k}, \mathbf{k}') = \frac{\delta^2 E_0}{\delta n(\mathbf{k}) \delta n(\mathbf{k}')}$$

At the Fermi surface this is an exact relation.

The structure of the nucleon-nucleon interaction

Like the Skyrme force, the Migdal force is an expansion in momentum space. However, contrary to HF potentials (such as the Skyrme force), the p^2-terms do not play an essential role. In most calculations it is therefore sufficient to take into account only the constant in momentum space which gives a pure δ-force in coordinate space. On the other hand, spin and isospin exchange mixtures are very important.

$$V(1,2) = V_0\delta(\mathbf{r}_1 - \mathbf{r}_2)(f + f'\boldsymbol{\tau}^{(1)}\boldsymbol{\tau}^{(2)} + g\boldsymbol{\sigma}^{(1)}\boldsymbol{\sigma}^{(2)} + g'\boldsymbol{\sigma}^{(1)}\boldsymbol{\sigma}^{(2)}\boldsymbol{\tau}^{(1)}\boldsymbol{\tau}^{(2)})$$

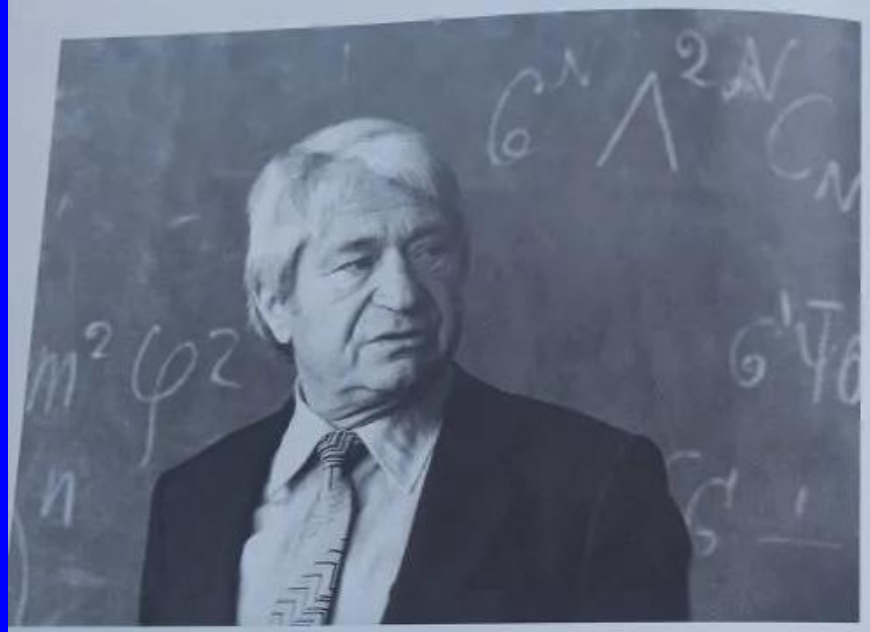
Guman and Birbrair proposed to take into account the different interaction strengths inside and outside the nucleus and the diffuseness of the nuclear surface by a linear density dependence of the parameters f and f'

$$f = f^{ex} + (f^{in} - f^{ex})\rho(r)$$

where $\rho(r)$ has the form of a Fermi distribution

$$\rho(r) = \frac{1}{1 + \exp[(r - R)/a]}$$

In contrast to a Hartree-Fock calculation with a density dependent interaction, the density is not adjusted self-consistently. The Migdal force has been widely used to calculate collective vibrations in nuclei. The vibrations provide the experimental data with which to adjust the six parameters f_{in} f_{ex} f'_{in} f'_{ex} g g'



А.Мигдал

ВОСПОМИНАНИЯ ОБ АКАДЕМИКЕ А.Б. Мигдале

МОСКВА
ФИЗМАТЛИТ
2003

The Skyrme energy density functional and the Hartree-Fock equations

We start with the Skyrme force

$$v_{12} = t_0(1 + x_0 P_\sigma)\delta(\vec{r}_1 - \vec{r}_2)$$
$$+ \tfrac{1}{2} t_1[\delta(\vec{r}_1 - \vec{r}_2)k^2 + k'^2\delta(\vec{r}_1 - \vec{r}_2)]$$
$$+ t_2\vec{k}' \cdot \delta(\vec{r}_1 - \vec{r}_2)\vec{k} + iW_0(\vec{\sigma}_1 + \vec{\sigma}_2) \cdot \vec{k}' \times \delta(\vec{r}_1 - \vec{r}_2)\vec{k}$$
$$V(1,2,3) = t_3\delta(\mathbf{r}_1 - \mathbf{r}_2)\delta(\mathbf{r}_2 - \mathbf{r}_3)$$

where $\vec{k}$ now denotes the operator $(\vec{\nabla}_1 - \vec{\nabla}_2)/2i$ acting on the right; whereas, $\vec{k}'$ is the operator $-(\vec{\nabla}_1 - \vec{\nabla}_2)/2i$ acting on the left.

The expectation value of the energy is given by

$$E = \langle \phi, (T + V)\phi \rangle$$
$$= \sum_i \left\langle i \left| \frac{p^2}{2m} \right| i \right\rangle + \frac{1}{2}\sum_{ij} \langle ij|\, \bar{v}_{12}|ij\rangle$$
$$+ \frac{1}{6}\sum_{ijk} \langle ijk|\, \bar{v}_{123}|ijk\rangle$$
$$= \int H(\vec{r})\, d^3r\,,$$

where the notation $\bar{v}$ denotes an antisymmetrized matrix element. For the Skyrme interaction the energy density $H(\vec{r})$ is an algebraic function of the nucleon densities $\rho_n(\rho_p)$, the kinetic energy τ_n (τ_p), and spin densities $\vec{J}_n$ $(\vec{J}_p)$.

$$\rho_q(\vec{r}) = \sum_{i,\sigma} |\, \phi_i(\vec{r}, \sigma, q)|^2\,,$$

$$\tau_q(\vec{r}) = \sum |\, \vec{\nabla}\phi_i(\vec{r}, \sigma, q)|^2\,,$$

$$\vec{J}_q(\vec{r}) = (-i) \sum_{i,\sigma,\sigma'} \phi_i^*(\vec{r}, \sigma, q)[\, \vec{\nabla}\phi_i(\vec{r}, \sigma', q) \times \langle \sigma|\vec{\sigma}|\sigma'\rangle]$$

$$H(\vec{r}) = \frac{\hbar^2}{2m}\tau(\vec{r}) + \tfrac{1}{2}t_0[(1 + \tfrac{1}{2}x_0)\rho^2 - (x_0 + \tfrac{1}{2})(\rho_n^2 + \rho_p^2)] + \tfrac{1}{4}(t_1 + t_2)\rho\tau + \tfrac{1}{8}(t_2 - t_1)(\rho_n\tau_n + \rho_p\tau_p) + \tfrac{1}{16}(t_2 - 3t_1)\rho\nabla^2\rho$$
$$+ \tfrac{1}{32}(3t_1 + t_2)(\rho_n\nabla^2\rho_n + \rho_p\nabla^2\rho_p) + \tfrac{1}{16}(t_1 - t_2)(\vec{J}_n^2 + \vec{J}_p^2) + \tfrac{1}{4}t_3\rho_n\rho_p\rho + H_C(\vec{r}) - \tfrac{1}{2}W_0(\rho\vec{\nabla}\cdot\vec{J} + \rho_n\vec{\nabla}\cdot\vec{J}_n + \rho_p\vec{\nabla}\cdot\vec{J}_p)$$

The Skyrme energy density functional and the Hartree-Fock equations

$$H(\vec{r}) = \frac{\hbar^2}{2m}\tau(\vec{r}) + \tfrac{1}{2}t_0[(1+\tfrac{1}{2}x_0)\rho^2 - (x_0+\tfrac{1}{2})(\rho_n^2+\rho_p^2)] + \tfrac{1}{4}(t_1+t_2)\rho\tau + \tfrac{1}{8}(t_2-t_1)(\rho_n\tau_n+\rho_p\tau_p) + \tfrac{1}{16}(t_2-3t_1)\rho\nabla^2\rho$$

$$+\tfrac{1}{32}(3t_1+t_2)(\rho_n\nabla^2\rho_n+\rho_p\nabla^2\rho_p) + \tfrac{1}{16}(t_1-t_2)(\vec{J}_n^{\,2}+\vec{J}_p^{\,2}) + \tfrac{1}{4}t_3\rho_n\rho_p\rho + H_C(\vec{r}) - \tfrac{1}{2}W_0(\rho\vec{\nabla}\cdot\vec{J}+\rho_n\vec{\nabla}\cdot\vec{J}_n+\rho_p\vec{\nabla}\cdot\vec{J}_p)$$

In a nucleus with N=Z and no Coulomb field we have $\rho_n = \rho_p = \frac{1}{2}\rho, \quad \tau_n = \tau_p = \frac{1}{2}\tau, \quad \vec{J}_n = \vec{J}_p = \frac{1}{2}\vec{J}$

The EDF expression simplifies to

$$H(\vec{r}) = \frac{\hbar^2}{2m}\tau + \tfrac{3}{8}t_0\rho^2 + \tfrac{1}{16}t_3\rho^3 + \tfrac{1}{16}(3t_1+5t_2)\rho\tau$$

$$+\tfrac{1}{64}(9t_1-5t_2)(\vec{\nabla}\rho)^2 - \tfrac{3}{4}W_0\rho\vec{\nabla}\cdot\vec{J}.$$

In nuclear matter $\vec{\nabla}\rho = \vec{\nabla}\cdot\vec{J} = 0$ we have translational invariance and the single-particle wave functions are given by plane waves

$$\varphi_{ksi} = \frac{1}{(2\pi)^{3/2}}e^{ikr}\chi_s^{1/2}\chi_i^{1/2}$$

we have to replace $\sum_{i=1}^{A}\ldots$ by $\int_{|k|<k_F} d^3k\ldots$

where all the levels with k smaller than the Fermi momentum are occupied. We get the usual relations

$$\rho = \frac{4}{(2\pi)^3}\frac{4\pi}{3}k_F^3 = \frac{2}{3\pi^2}k_F^3$$

$$\tau = \frac{2}{3\pi^2}\frac{3}{5}k_F^5 = \frac{3}{5}\rho k_F^2 = \frac{3}{5}\left(\frac{3\pi^2}{2}\right)^{2/3}\rho^{5/3}$$

D. VAUTHERIN AND D. M BRINK

PHYSICAL REVIEW C VOLUME 5, NUMBER 3 MARCH 1972

The Skyrme energy density functional and the Hartree-Fock equations

We obtain the binding energy per particle in nuclear mater

$$\frac{E_0}{A}=\frac{H}{\rho}=\frac{3}{5}\frac{\hbar^2}{2m}k_F^2+\frac{3}{8}t_0\rho+\frac{1}{16}t_3\rho^2+\frac{3}{80}(3t_1+5t_2)\rho k_F^2$$

The saturation property means that there is an equilibrium density ρ_0

$$\left.\frac{\partial}{\partial\rho}\left(\frac{E_0}{A}\right)\right|_{\rho=\rho_0}=0=\frac{2}{5}\frac{\hbar^2}{2m}k_F^2\rho^{-1}+\frac{3}{8}t_0+\frac{1}{8}t_3\rho+\frac{1}{16}(3t_1+5t_2)k_F^2.$$

The incompressibility of nuclear matter K is defined as the curvature of the binding energy with respect to the Fermi momentum

$$K=k_F^2\left.\frac{\partial^2(E_0/A)}{\partial k_F^2}\right|_{\rho=\rho_0}=\frac{6}{5}\frac{\hbar^2}{2m}k_F^2+\frac{9}{4}t_0\rho+\frac{15}{8}t_3\rho^2+\frac{3}{4}(3t_1+5t_2)\rho k_F^2$$

These equations allow us to express the $t_0, t_3, 3t_1+5t_2$ by the nuclear matter properties E_0/A, ρ_0 and K. We see that t_3 is strongly correlated with the incompressibility K. From the Bethe-Weizsäcker formula, we know that E_0/A =15.9 MeV. Less well determined is the equilibrium density ρ_0=0.16fm^{-3}. Therefore, it is not possible to adjust the EDF parameters to nuclear matter data alone. We first have to carry out the calculation for finite nuclei.

The Skyrme energy density functional and the Hartree-Fock equations

We derive the density dependent Hartree-Fock equations. We have to vary the EDF with respect to the densities in order to gain the Hartree-Fock Hamiltonian. Unfortunately, the EDF does not have the form of a functional of ρ . It also depends on τ and J . In our case this is no real problem, since the HF-densities are defined by the single-particle wave functions φ_l .We use Lagrange multipliers ϵ_l for these subsidiary conditions

$$\frac{\delta}{\delta\varphi_k}\left(E_0[\rho]-\sum_l \epsilon_l \int d^3r|\varphi_l(\mathbf{r})|^2\right)=0$$

The variation of the energy can be written

$$\delta E=\int d^3r\left[\frac{\hbar^2}{2m^*(\mathbf{r})}\delta\tau(\mathbf{r})+U(\mathbf{r})\delta\rho(\mathbf{r})+\mathbf{W}(\mathbf{r})\delta\mathbf{J}(\mathbf{r})\right]$$

After integrating by parts, we get

$$\delta E=2\sum_{i=1}^{A}\int d^3r\,\delta\varphi_i^*\left\{-\nabla\frac{\hbar^2}{2m_\tau^*}\nabla+U+\mathbf{W}\frac{1}{i}(\nabla\times\sigma)\right\}\varphi_i$$

We finally find the HF-equation in coordinate space

$$\left\{-\nabla\frac{\hbar^2}{2m^*(\mathbf{r})}\nabla+U(\mathbf{r})+\mathbf{W}\frac{1}{i}(\nabla\times\sigma)\right\}\varphi_i(\mathbf{r})=\epsilon_i\varphi_i(\mathbf{r})$$

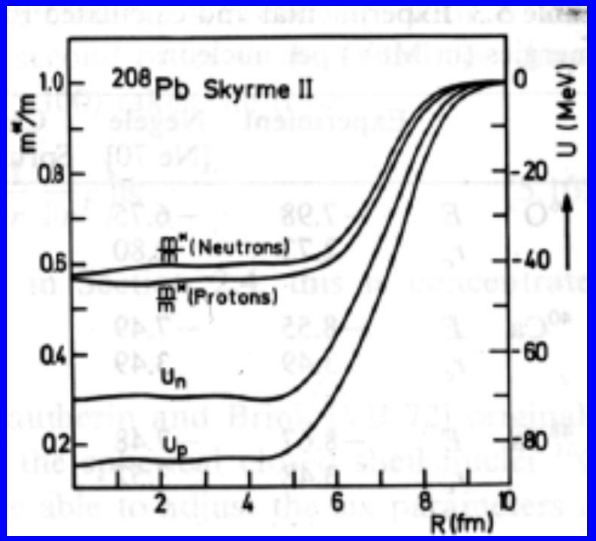
The Skyrme energy density functional and the Hartree-Fock equations

$$\left\{ -\nabla \frac{\hbar^2}{2m^*(\mathbf{r})} \nabla + U(\mathbf{r}) + \mathbf{W} \frac{1}{i} (\nabla \times \boldsymbol{\sigma}) \right\} \varphi_i(\mathbf{r}) = \epsilon_i \varphi_i(\mathbf{r})$$

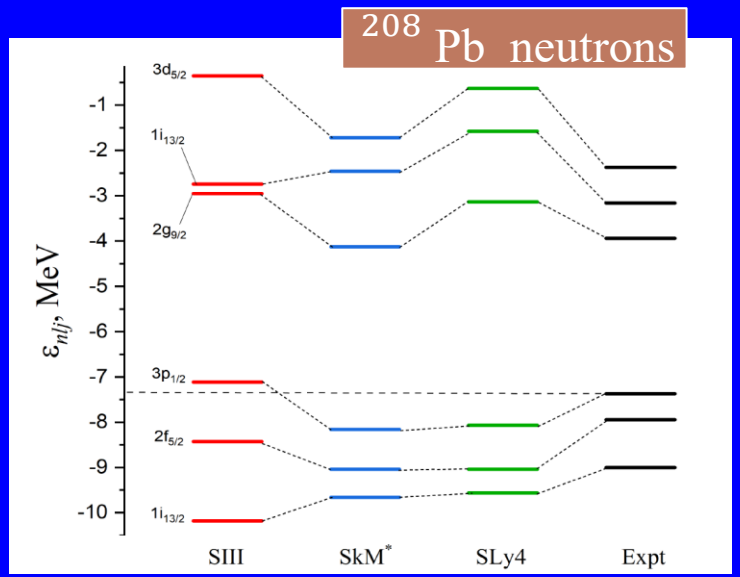
$$m^*(\mathbf{r}) = m\left(1 + \frac{2m}{\hbar^2}\frac{1}{16}(3t_1 + 5t_2)\rho\right)^{-1}$$

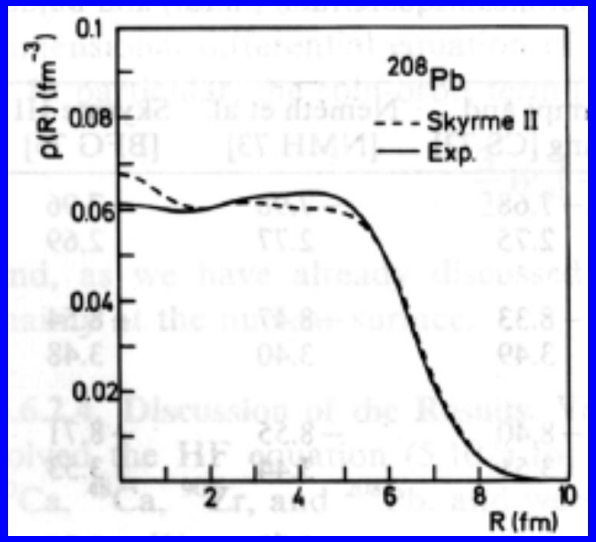
$$U(\mathbf{r}) = \frac{3}{4}t_0\rho + \frac{3}{16}t_3\rho^2 + \frac{1}{16}(3t_1 + 5t_2)\tau + \frac{1}{32}(5t_2 - 9t_1)\nabla^2\rho - \frac{3}{4}W_0\nabla \mathbf{J},$$

$$\mathbf{W}(\mathbf{r}) = \frac{3}{4}W_0\nabla\rho$$



With increasing effective mass, we obtain a compression of the spectrum





The Skyrme energy density functional and the Hartree-Fock equations

		Experiment	Negele [Ne 70]	Campi and Sprung [CS 72]	Nemeth et al. [NMH 73]	Skyrme III [BFG 75]
^{16}O	E	−7.98	−6.75	−7.68	−7.98	−7.96
	r_c	2.73	2.80	2.75	2.77	2.69
^{40}Ca	E	−8.55	−7.49	−8.33	−8.47	−8.54
	r_c	3.49	3.49	3.49	3.40	3.48
^{48}Ca	E	−8.67	−7.48	−8.40	−8.55	−8.71
	r_c	3.48	3.52	3.51	3.44	3.53
^{90}Zr	E	−8.71	−7.85	−8.63	−8.70	−8.71
	r_c	4.23	4.25	4.27	4.13	4.32
^{208}Pb	E	−7.87	−7.53	−7.87	−7.87	−7.87
	r_c	5.50	5.44	5.45	5.22	5.57

The Skyrme energy density functional and the Hartree-Fock equations

We discuss the basic references of the fitting protocol for EDF parameters

SI-SVI (Beiner *et al.*, 1975)	
E:	^{16}O, ^{40}Ca, ^{48}Ca, ^{56}Ni, ^{90}Zr, ^{140}Ce, ^{208}Pb
r:	^{16}O, ^{40}Ca, ^{48}Ca, ^{56}Ni, ^{90}Zr, ^{140}Ce, ^{208}Pb
$\ell \cdot \mathbf{s}$	^{16}O$(1p_n, 1p_p)$
	Additionally for SkM (Krivine *et al.*, 1980)
INM	K_∞, $a_{\rm sym}$ ($\leftrightarrow$ resonances in ^{208}Pb)
	Additionally for SkM* (Bartel *et al.*, 1982)
INM	$a_{\rm surf}$ ($\leftrightarrow$ fission barriers)

SLy1-10 (Chabanat *et al.*, 1998)	
% E:	^{16}O, ^{40}Ca, ^{48}Ca, ^{56}Ni, ^{78}Ni, ^{132}Sn, ^{208}Pb
% r:	^{16}O, ^{40}Ca, ^{48}Ca, ^{56}Ni, ^{208}Pb
$\ell \cdot \mathbf{s}$	^{208}Pb$(3p_n)$
INM	$(E/A)_{0,\rm eq}$, $\rho_{0,\rm eq}$, K_∞, $a_{\rm sym}$, $\kappa_{\rm TRK}$, EoS$_{\rm neut}$

The Skyrme energy density functional and the Hartree-Fock equations

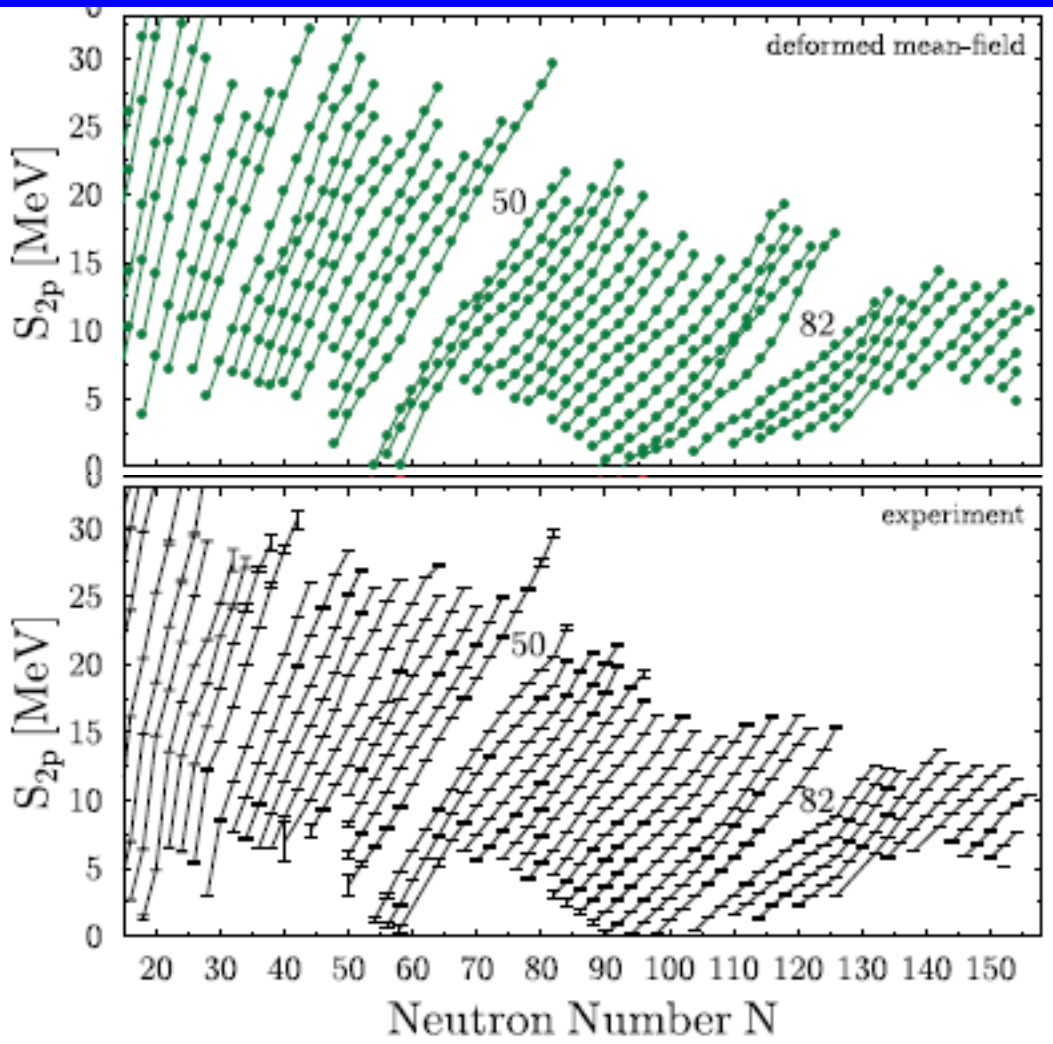


FIG. 3. (Color online) Two proton-separation energy S_{2p} for even-even nuclei. Lines connect nuclei in isotonic chains.

The Skyrme energy density functional and the Hartree-Fock equations

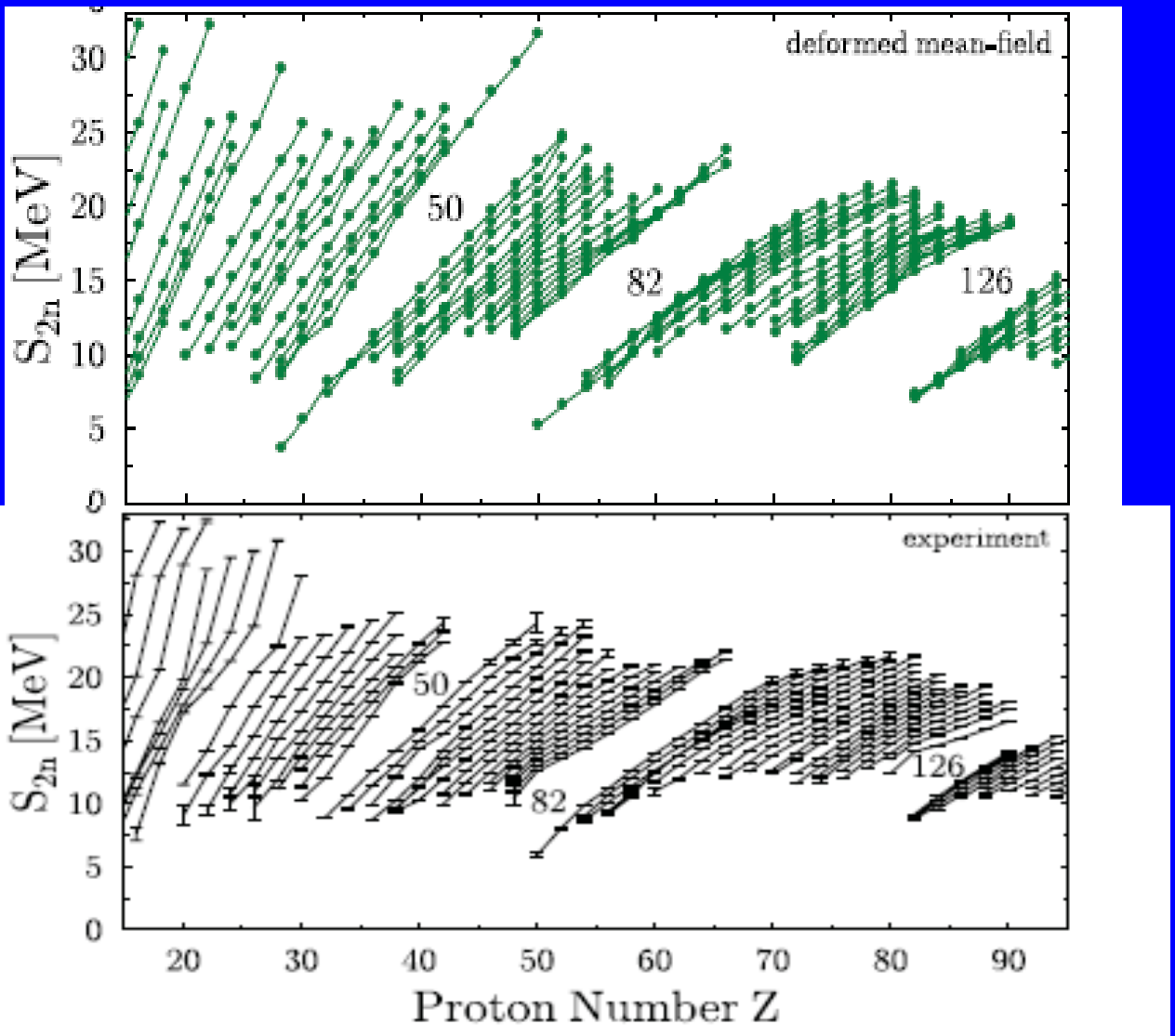
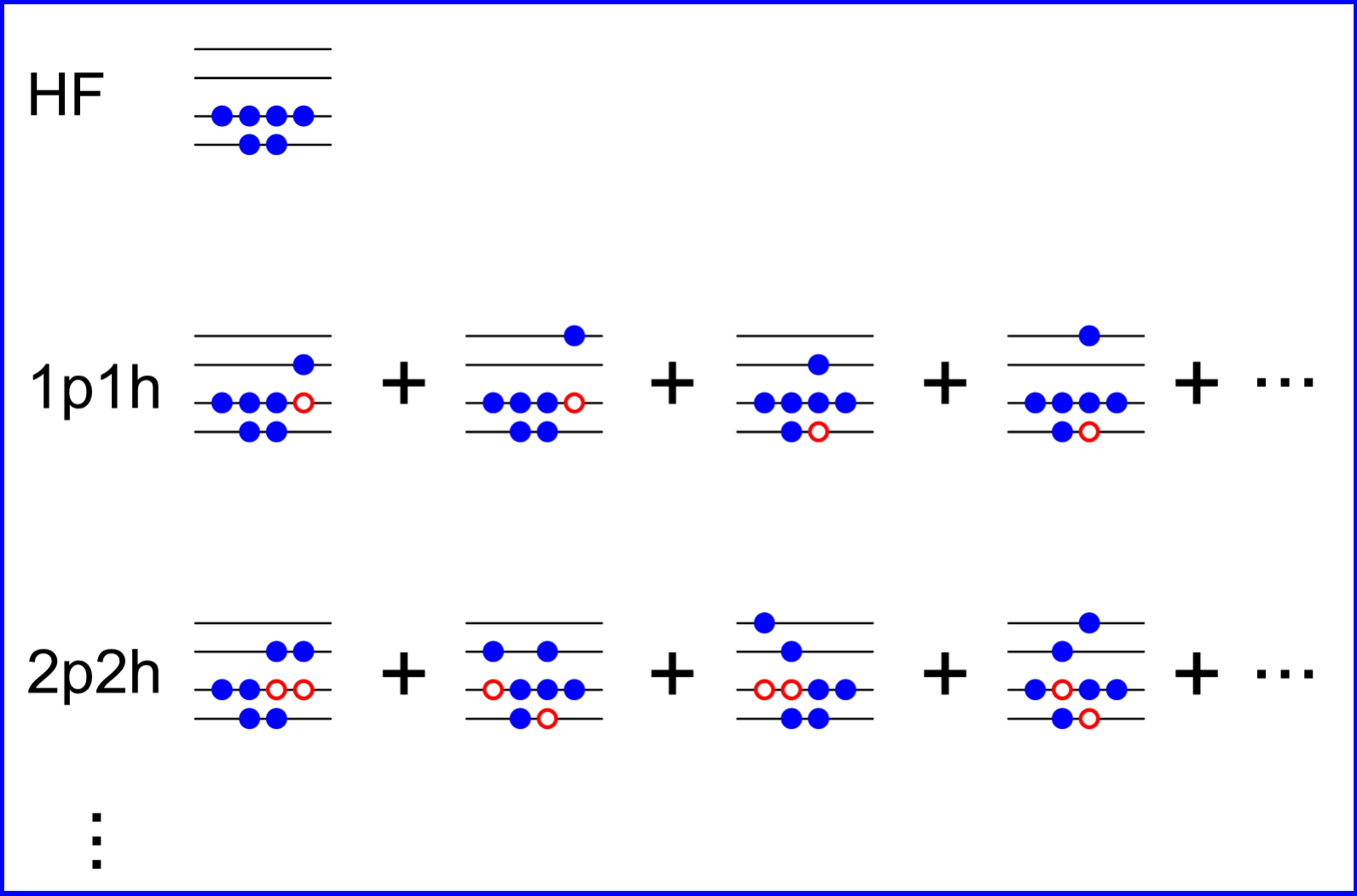


FIG. 4. (Color online) Two-neutron separation energy S_{2n} for even-even nuclei. Lines connect nuclei in isotopic chains.

Applications of Skyrme EDF to nuclear spectroscopy

Excited Nuclei



Applications of Skyrme EDF to nuclear spectroscopy

We introduce the phonon creation operators

$$Q^{+}_{\lambda\mu i} = \frac{1}{2}\sum_{jj'}\left(X^{\lambda i}_{jj'}\, A^{+}(jj';\lambda\mu) - (-1)^{\lambda-\mu} Y^{\lambda i}_{jj'}\, A(jj';\lambda-\mu)\right)$$

$$A^{+}(jj';\lambda\mu) = \sum_{mm'} \langle jmj'm' \mid \lambda\mu\rangle \alpha^{+}_{jm}\alpha^{+}_{j'm'}$$

One assumes that the QRPA ground state is the phonon vacuum $\mid 0\rangle$ $\quad Q_{\lambda\mu i}\mid 0\rangle = 0$

We define the excited states by $\quad Q^{+}_{\lambda\mu i}\mid 0\rangle$

QRPA equations

$$\begin{pmatrix} \mathcal{A} & \mathcal{B} \\ -\mathcal{B} & -\mathcal{A} \end{pmatrix}\begin{pmatrix} X \\ Y \end{pmatrix} = w \begin{pmatrix} X \\ Y \end{pmatrix}$$

Solutions of this set of linear equations yield the eigenenergies and the amplitudes X, Y of the excited states.
A dimension of the matrices $\mathcal{A}, \mathcal{B}$ is a space size of the two-quasiparticle configurations.

Applications of Skyrme EDF to nuclear spectroscopy

The coupling between one-, two- and three-phonon terms in the wave functions of excited states are taken into account

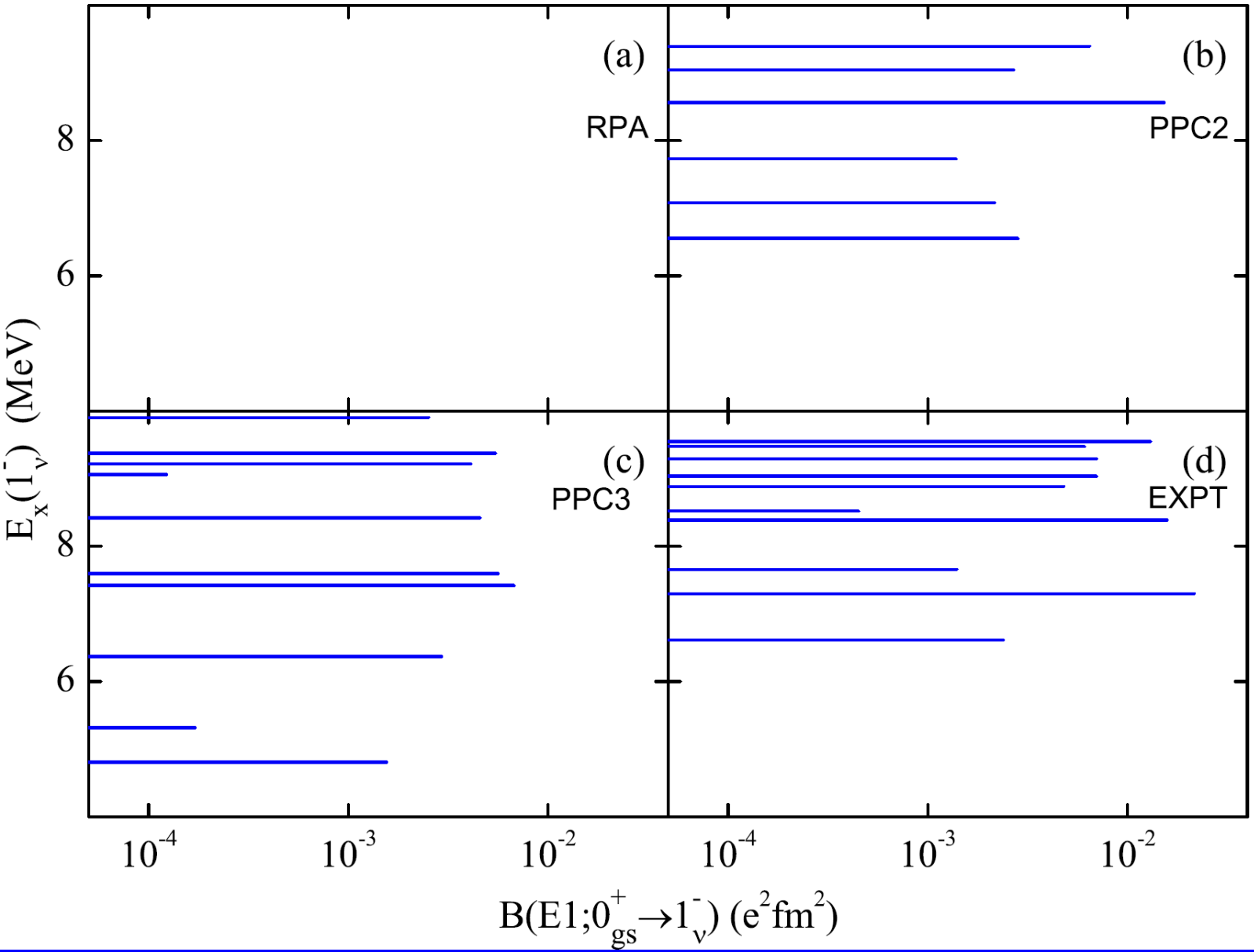
$$\Psi_\nu(JM) = \Bigg(\sum_i R_i(J\nu) Q^+_{JMi} + \sum_{\substack{\lambda_1 i_1 \\ \lambda_2 i_2}} P^{\lambda_1 i_1}_{\lambda_2 i_2}(J\nu) \left[Q^+_{\lambda_1 i_1} Q^+_{\lambda_2 i_2} \right]_{JM} + \sum_{\substack{\lambda_1 i_1 \\ \lambda_2 i_2 \\ \lambda_3 i_3 J'}} T^{\lambda_1 i_1 \, \lambda_2 i_2}_{J' \, \lambda_3 i_3}(J\nu) \left[\left[Q^+_{\lambda_1 i_1} Q^+_{\lambda_2 i_2} \right]_{J'} Q^+_{\lambda_3 i_3} \right]_{JM} \Bigg) |0\rangle$$

The equations have the same form as the equations of the quasiparticle-phonon model (QPM), but the single-particle spectrum and the parameters of the residual interaction are calculated with the Skyrme EDF.

A.P. Severyukhin, V.V. Voronov, and Nguyen Van Giai, Eur. Phys. J. A22, 397 (2004).

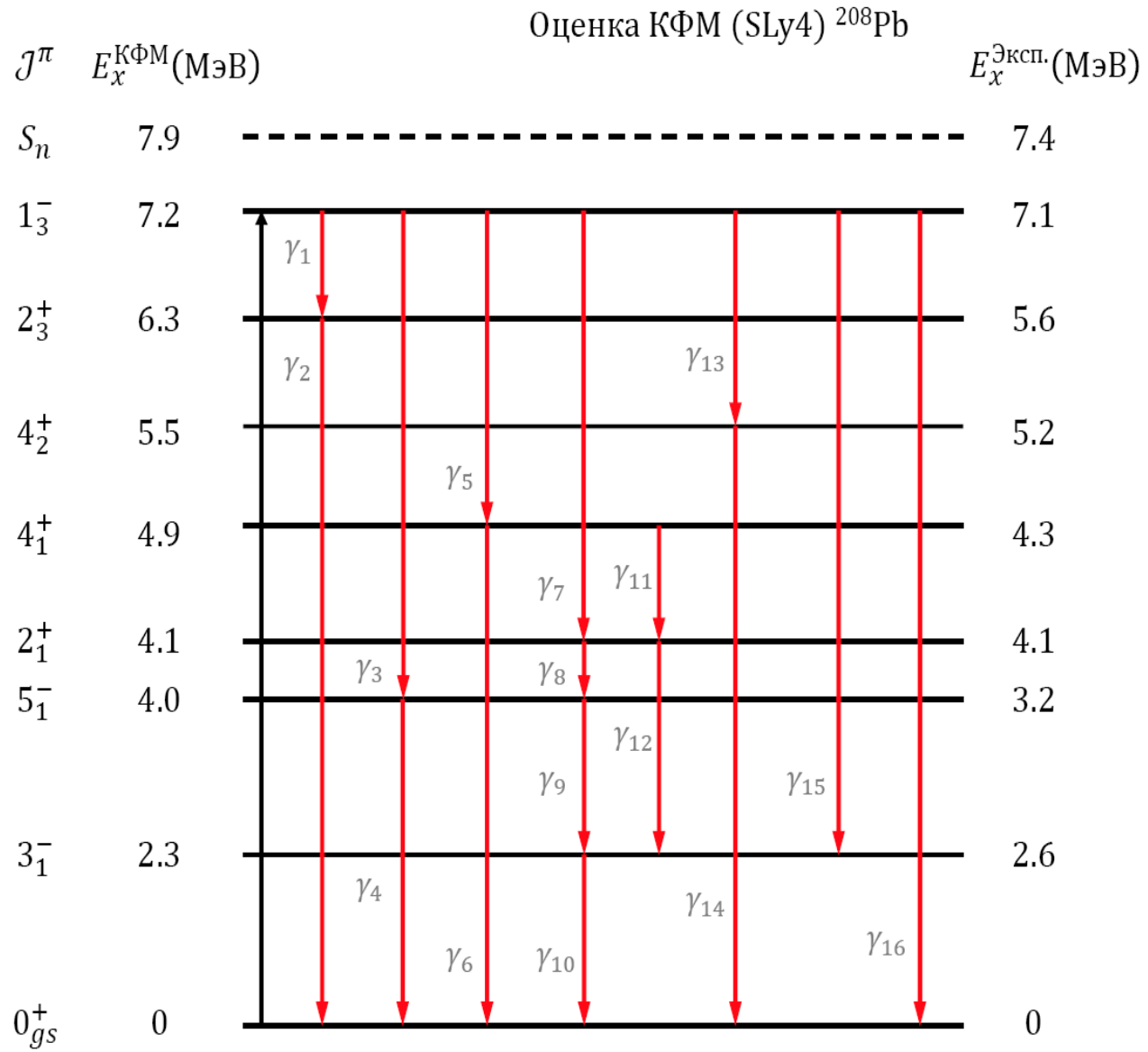
A.P. Severyukhin, N.N. Arsenyev, N. Pietralla, PRC 104, 024310 (2021).

Applications of Skyrme EDF to nuclear spectroscopy



A.P. Severyukhin, N.N. Arsenyev, N. Pietralla, PRC 104, 024310 (2021).

Applications of Skyrme EDF to nuclear spectroscopy

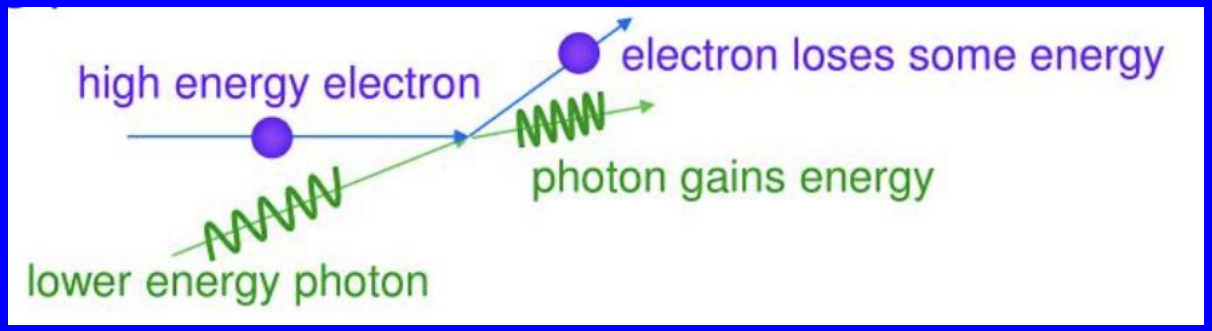


	КФМ	Эксп.
E_{γ_1}	0.9 МэВ	1.5 МэВ
E_{γ_2}	6.3 МэВ	5.6 МэВ
E_{γ_3}	3.2 МэВ	3.9 МэВ
E_{γ_4}	4.0 МэВ	3.2 МэВ
E_{γ_5}	2.2 МэВ	2.8 МэВ
E_{γ_6}	4.9 МэВ	4.3 МэВ
E_{γ_7}	3.1 МэВ	3.0 МэВ
E_{γ_8}	0.1 МэВ	0.9 МэВ
E_{γ_9}	1.7 МэВ	0.6 МэВ
$E_{\gamma_{10}}$	2.3 МэВ	2.6 МэВ
$E_{\gamma_{11}}$	0.8 МэВ	0.2 МэВ
$E_{\gamma_{12}}$	1.8 МэВ	1.5 МэВ
$E_{\gamma_{13}}$	1.7 МэВ	1.9 МэВ
$E_{\gamma_{14}}$	5.5 МэВ	5.2 МэВ
$E_{\gamma_{15}}$	4.9 МэВ	4.5 МэВ
$E_{\gamma_{16}}$	7.2 МэВ	7.1 МэВ

M. S. Kosarev, N.N. Arsenyev, A.P. Severyukhin, in preparation

Applications of Skyrme EDF to nuclear spectroscopy

Inverse compton scattering for new γ beam facilities



- **High Intensity γ-ray Source (HIγS)**
- **Extreme Light Infrastructure – Nuclear Physics (ELI-NP)**
- **Shanghai Laser Electron Gamma Source (SLEGS)**
- **ИКИ НЦФМ**

Thank you for your kind attention!