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Structure models: from shell models to ab-initio methods

Shell Model

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EXOTIC 2015: Re-writing Nuclear Physics textbooks

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Friday, 17 July, 15



Content

- Evidence of shells in nuclei
- Representation of a many body wave function
- Non interacting shell model
- Interacting shell model
- "Ab-initio" shell model
- Ab-initio methods
- Hyperspherical harmonic expansions
- Lorentz Integral transform
- Coupled-cluster theory
- Selected applications in the physics of exotic nuclei



Nuclear Theory

Our Goal

Develop a unified theory of all nuclei in the nuclear chart



Connecting to QCD

Connecting to Astrophysics

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



Shell Model in Atoms

Electrons in atoms occupy well defined shells of discrete, well separated energies.



Evidence of electron shells in atoms: sudden jumps in atomic properties as the shell gets filled up, such as atomic radius, ionization energy etc.



Shell Model in Atoms



Do nucleons inside the nucleus do the same or not?

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Shell Model in Nuclei?

Shell structure in the nucleus would mean that individual nucleons inhabit orbitals of well defined energy. Not evident a priory why this should be the case. Why?

• The liquid drop model (smooth) is very successful in describing the binging energy.



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Shell Model in Nuclei?

Shell structure in the nucleus would mean that individual nucleons inhabit orbitals of well defined energy. Not evident a priory why this should be the case. Why?

- The liquid drop model (smooth) is very successful in describing the binging energy.
- No obvious centre for nucleons to orbit around.
- No external potential in nuclei, that should be the equivalent of the Coulomb force in atoms.

But the experimental evidence seems to say otherwise!

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Shell Model in Nuclei?



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Nuclei exhibit a shell structure! Experimental data indicate local maxima of the binding energy and local minima of radii in proximity of the neutron or proton "magic numbers" 2, 8, 20,28, 50, 82, 126

We are physicists, so we do not believe in magic! Where do these magic numbers come from? They have to be related to the way nucleons interact with each other.

The theory that explains this is called non interacting shell model or nuclear shell model. It is a simplified theory that accounts though for measured properties and can predict others. It is based on the assumption that the motion of the single nucleon is governed by a potential caused by all other nucleons.

In order to understand where the magic numbers come from and to explain the theory of the nuclear shell model, we need to open a parenthesis on:

- how to represent a many-body wave function
- what is an independent particle model

 In order to construct a many-body wave function, one first has to start from a single particle (nucleon) wave function, which is separated in space/spin/isospin components

$$\left\langle arphi_k
ight
angle = \left[\left| arphi_k^{space}
ight
angle \otimes \left| arphi_k^{spin}
ight
angle
ight] \otimes \left| arphi_k^{isospin}
ight
angle$$

This could be the solution of the single nucleon Schrödinger equation

 $h|arphi_k
angle=arepsilon_k|arphi_k
angle$ (\$



One can then use these single particle states to construct a many-body wave function.
 The many-body space is in general the product of many single particle Hilbert spaces

$$H^A = h_1 \otimes h_2 \otimes \cdots \otimes h_A$$

Each single particle state is spanned by $\{|\varphi_k\rangle\}$ as solution of (\Rightarrow)

 We can construct a many-body wave function as the product of single particle wave functions that each live in their own single particle Hilbert space



The symbol \otimes is for an ordered product, which means if you exchange the index 1 with the index 2 you have a different w.f.

```
|\varphi_{k_1}\rangle\otimes|\varphi_{k_2}\rangle\neq|\varphi_{k_2}\rangle\otimes|\varphi_{k_1}\rangle,
```

The first position refers to the first particle, the second position refers to the second particle and so on...

Since we deal with identical particles which are fermions, we need to work with many-body states that are antisymmetrized with respect to the exchange of two particles

Antisymmetrized many-body wave function

 $|\psi^{A}\rangle = \mathcal{A}\left\{|\varphi_{k_{1}}\rangle\otimes|\varphi_{k_{2}}\rangle\otimes\cdots\otimes|\varphi_{k_{A}}\rangle\right\}$

where the antisymmetrizer operator is



where P_P is the permutation operator

 $sign(P) = (-1)^{n_p}, n_p$: number of pair exchanges

Example of permutations with A=3 (A!=6)



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• The Hamiltonian always commute with the antisymmetrization operator [H, A] = 0(the Hamiltonian is always written in a symmetric form) As a consequence they can have the same eigenvectors

$$|\psi^A\rangle = \mathcal{A}\left\{|\varphi_{k_1}\rangle \otimes |\varphi_{k_2}\rangle \otimes \cdots \otimes |\varphi_{k_A}\rangle\right\}$$

Slater Determinant:

antisymmetrized product of single particle states

Imposing antisymmetrization means respecting Pauli principle \rightarrow If we put two particle in the same state, when we permute, the antisymmetrizer will give zero.

Example A=2

Suppose we neglect spin-isospin now and use a coordinate representation of the single particle states, i.e., $\langle r|\varphi_k\rangle = \varphi_k(r)$

$$\begin{aligned} \langle r_1 | \otimes \langle r_2 | \mathcal{A} \{ | \varphi_{k_1} \rangle \otimes | \varphi_{k_2} \rangle \} &= \langle r_1 | \otimes \langle r_2 | (| \varphi_{k_1} \rangle \otimes | \varphi_{k_2} \rangle - | \varphi_{k_2} \rangle \otimes | \varphi_{k_1} \rangle) \frac{1}{2} \\ &= \frac{1}{2} (\varphi_{k_1}(r_1) \varphi_{k_2}(r_2) - \varphi_{k_2}(r_1) \varphi_{k_1}(r_2)) = \frac{1}{2} \det \begin{pmatrix} \varphi_{k_1}(r_1) & \varphi_{k_1}(r_2) \\ \varphi_{k_2}(r_1) & \varphi_{k_2}(r_2) \end{pmatrix} \\ &\uparrow \end{aligned}$$

here particle one is in state k_2

Case of A particles coordinate space representation

Slater Determinant

$$\langle r_1, r_2, \dots, r_A | \psi^A \rangle = \frac{1}{A!} \det \left(\begin{array}{ccc} \varphi_{k_1}(r_1) & \varphi_{k_1}(r_2) & \cdots & \varphi_{k_1}(r_A) \\ \vdots & \vdots & \ddots & \vdots \\ \varphi_{k_A}(r_1) & \varphi_{k_A}(r_2) & \cdots & \varphi_{k_A}(r_A) \end{array} \right)$$

Determinant of an AxA matrix, with same particle in each column and same single particle state in each row.

It is a (simple) way to construct antisymmetrized states.

Exercise: Play with the three-particle Slater Determinant.

Independent particle model

In an independent particle model it is assumed that particles do not interact with each other. They are only subject to the Pauli principle.

Formally this means that one can write the Hamiltonian for A particles as

$$H = \sum_{i=1}^{N} h_i$$
, h_i : single particle Hamiltonian

Note: there is nothing that connects particle i with particle j

Examples:

$$h_i = \frac{p_i^2}{2m}$$
 only kinetic energy (Fermi gas models with SD of plane waves)

$$h_i = \frac{p_i^2}{2m} + U_i$$

 U_i is the potential felt by particle i, which could be an external potential like the Coulomb force in atoms or an average potential given to *i* by the presence of all the other A-1 particles.

Assumption: The interaction of a nucleon with ALL the other particles is approximated by a "mean" potential



Independent particle model

$$\begin{split} H &= \sum_{i}^{A} h_{i} \quad \text{The solution of such Hamiltonian is obtained by solving the} \\ h_{i} |\varphi_{k}\rangle &= \varepsilon_{k} |\varphi_{k}\rangle \implies h_{i} \varphi_{k}(r_{i}) = \varepsilon_{k} \varphi_{k}(r_{i}) \quad \text{ in coordinate space representation} \\ \text{Then the A-body states are just Slater Determinants of single particle states} \quad \varphi_{k}(r_{i}) \quad \text{The solution of} \quad H |\psi^{A}\rangle = E |\psi^{A}\rangle \quad \text{has the following energy} \end{split}$$

 $E = \sum_{k}^{A} \varepsilon_{k} \overline{d_{k}} \longrightarrow$ degeneracy: measures the occupancy of a single particle state

Exercise: To convince yourself, prove that this is true for A=2

Independent particle model



Magic numbers arise because the single particle spectrum is not smooth, but is made by discrete levels. Particles are grouped into shells with relatively large gaps between them.



Separation Energies



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Structure models: from shell model to ab-initio methods

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Case of the spherical HO potential

$$U_{i} = \frac{1}{2}m\omega^{2}r_{i}^{2} \implies h_{i} = \frac{p_{i}^{2}}{2m} + \frac{1}{2}m\omega^{2}r_{i}^{2}$$
$$h_{i} \varphi(\vec{r}_{i}) = \varepsilon_{k} \varphi(\vec{r}_{i}) \qquad \text{HO in 3 dimensions}$$

HO in 3 dimensions

- bunch of quantum numbers $k = n\ell m$ k

For every particle (omit *i* index)

$$\varphi_{n\ell m}(\vec{r}\) = R_{n\ell}(r) Y_{\ell m}(\hat{r})$$

$$n \quad \text{radial quantum number}$$

$$n \quad \text{radial quantum numbers related to}$$

$$n \quad \text{quantum numbe$$

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Structure models: from shell model to ab-initio methods



Case of the spherical HO potential



The integrated degeneracy is related to the magic numbers

Ν	E _N	d _N	$\sum_{N} d_{N}$	n(1)	parity
0	$\frac{3}{2}\hbar\omega$	2	2	15	+
1	$\frac{5}{2}\hbar\omega$	6	8	1 <i>p</i>	-
2	$\frac{7}{2}\hbar\omega$	12	20	1 <i>d</i> , 2 <i>s</i>	+
3	$\frac{9}{2}\hbar\omega$	20	40	1f, 2p	-
4	$\frac{11}{2}\hbar\omega$	30	70	1g, 2d, 3s	+
5	$\frac{13}{2}\hbar\omega$	42	112	1h, 2f, 3p	-
6	$\frac{15}{2}\hbar\omega$	56	168	1i, 2g, 3d, 4s	+

The magic numbers are wrong after the first three!



Does it depend on the "mean" potential we chose? We can do the same using a different U_i



Figure 5.4 Shell structure obtained with infinite well and harmonic oscillator potentials. The capacity of each level is indicated to its right. Large gaps occur between the levels, which we associate with closed shells. The circled numbers indicate the total number of nucleons at each shell closure.

Krane, Introductory Nuclear Physics



One can try to use a Wood-Saxton form for U_i



From Krane "Introductory Nuclear Physics"

Still the empirical magic number are not reproduced 2, 8, 20,28, 50, 82, 126

None of these single particle potentials seemed to work properly





Fermi's suggestion: any evidence for a spin-orbit force?

Mean field central potential plus an empirical spin-orbit term like

$$U(r) = V_0(r) + V_{\ell s}(r) \ \vec{\ell} \cdot \vec{s}$$

- $\vec{\ell}$ orbital angular momentum
- \vec{s} spin (intrinsic) angular momentum

with $V_0(r), V_{\ell s}(r)$ being negative (attractive potentials)





Spin-orbit splitting

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Now the good quantum numbers is j, so we have to consider the angular momentum coupling

$$\vec{j} = \vec{\ell} + \vec{s} = \vec{\ell} + \frac{\vec{1}}{2} = \begin{cases} j = \frac{3}{2} \\ j = \frac{1}{2} \end{cases} \quad \text{for } \ell = 1 \end{cases}$$



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With the addition of the spin-orbit, the magic numbers are reproduced 2, 8, 20, 28, 50, 82, 126 Intermediate



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Now we can build up the shell structure of nuclei like, just like we fill up the electron shells in atoms. Only now there are separate proton and neutron shells.



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Now we can build up the shell structure of nuclei like, just like we fill up the electron shells in atoms. Only now there are separate proton and neutron shells.



double closed s-shell

double closed p-shell

double magic nuclei: extra binding energy, extra small radius, extra low reaction probability





double closed sub-shell $p_{3/2}$ is full (6 p + 6 n)

closed p-shell for neutrons (8) closed p_{3/2} sub-shell for protons (6)

Protons and neutrons pair off, so that if there is an even number of p and n, then the total angular momentum of the nucleus in the g.s. is $J=0^+$



If there is an unpaired p or n, then the total angular momentum J^p of the nucleus in the g.s. is equal to the angular momentum and parity of the single nucleon in the outer shell



6 protons and 7 neutrons. One n in the outer p1/2 shell The nucleus has $J=1/2^{-1}$



If there is an unpaired p or n, then the total angular momentum J^p of the nucleus in the g.s. is equal to the angular momentum and parity of the single nucleon in the outer shell



6 protons and 5 neutrons. One unpaired n in the p3/2 shell, the nucleus has J=3/2⁻ A vacancy in an otherwise filled shell acts like a lone particle in that same shell in determining the spin parity of the nucleus. Thus, again, J=3/2⁻

Exercise: Give parity and J assignments of selected nuclei ...

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Interacting shell model

What we have described so far is known as non interacting shell model and we have discussed the ground state of nuclei.

However, in modern research what is used is the interacting shell model/shell model.

One can construct excited states or correlated ground states out of particle-hole excitations of the starting Slater determinant.



In this way you construct many Slater determinants, that can form a many-body basis which one can use to expand the many-body wave function. This is also called configuration mixing $|\Psi^A\rangle = \sum c_i |\psi_i^A\rangle$

Interacting shell model

Hamiltonian with a two-body potential (now particles are interacting)



So far we have not specified what the potentials are U_i, V_{ij}

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Interacting shell model

Construct orbitals from the HO potential

$$U_i = \frac{1}{2}m\omega^2 r_i^2 \qquad \hbar\omega \simeq 41A^{-\frac{1}{3}} \text{ MeV}$$

Ansatz:

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For a given number on p and n, the mean field orbitals can be grouped in:

- inherent core: orbitals that are always full
- valence space: orbits that can have particle-hole excitations
- external space: all the remaining orbits that are always empty
- 1. Starting from V_{ij} you construct a V^{eff}_{ij} that lives in the valence space using many body perturbation theory
- 2. Solve H₀+W_{res} by **diagonalizing** a matrix with particlehole excitations in your valence space





Diagonalization methods

Solve Schroedinger equation by expanding the w.f. on a set of basis states

$H \left \psi \right\rangle = E \left \psi \right\rangle$	$\ket{\psi} = \sum_{i}^{\infty} \stackrel{N}{c_i} \ket{\psi_i}$	 cannot store an → basis states: • f 	infinite vector ast convergence
N	$\frac{N}{\sum}$	•	arge model spaces
$\langle \psi_j \times H \sum_i c_i \psi_i \rangle$	$= E \sum_{i} c_i \psi_i\rangle$	• (different A
$\sum_{i=1}^{N} \langle \psi_{j} H \psi_{i} \rangle c_{i} = 1$	$E\sum_{i}^{N}c_{i}\left\langle \psi _{j} \psi _{i} ight angle$		
i $\sum_{H_{ji}}$	i δ_{ji}		
Hc =	Eigenva Hermiti	alue problem for an an matrix	$\mathbf{H}=\mathbf{H}^{\dagger}$

Finding eigenvalues and eigenvectors is equivalent to diagonalize the matrix N³ operation

Computationally challenging for growing N



Effective Potentials

The model space and the effective interaction are very much related. Typically, the effective interaction is a set of two-body matrix elements tuned to reproduce experimental data



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How to go beyond phenomenological potentials: a more fundamental approach to nuclear interactions

A more microscopic view on V_{ij}

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Structure models: from shell model to ab-initio methods



Nucleon-Nucleon Forces

one-pion

exchange potential (OPE)



exchange of massless particle

electromagnetic force:

infinite range





NN force: finite range exchange of massive particle



Hideki Yukawa Nobel prize in 1949

Realistic NN potentials: fit to NN scattering data with $\chi^2 pprox 1$





Chiral Effective Field Theory



Quark/gluon (high energy) dynamics

$$\mathcal{L} = -\frac{1}{4}G^a_{\mu\nu}G^{\mu\nu}_a + \bar{q}_L i\gamma_\mu D^\mu q_L + \bar{q}_R i\gamma_\mu D^\mu q_R - \bar{q}\mathcal{M}q$$

In the limit of vanishing quark masses the QCD Lagrangian is invariant under chiral symmetry

QCD chiral symmetry



Chiral symmetry is explicit and spontaneous broken





Nucleon/pion (low energy) dynamics

$$\mathcal{L}_{eff} = \mathcal{L}_{\pi\pi} + \mathcal{L}_{\pi N} + \mathcal{L}_{NN} + \dots$$

Compatible with explicit and spontaneous chiral symmetry breaking

Structure models: from shell model to ab-initio methods

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Chiral Effective Field Theory





Systematic expansion

 $\mathcal{L} = \sum_{\nu} c_{\nu} \left(\frac{Q}{\Lambda_b} \right)^{\nu}$

Limited resolution at low energy

Details of short distance physics not resolved, but captured in low energy constants (LEC)



Power counting

$$\nu = -4 + 2N + 2L + \sum_{i} (d_i + n_i/2 - 2)$$

Exercise on power counting.



Chiral Effective Field Theory





Systematic expansion

 $\mathcal{L} = \sum_{\nu} c_{\nu} \left(\frac{Q}{\Lambda_b} \right)^{\nu}$

Limited resolution at low energy

Details of short distance physics not resolved, but captured in low energy constants (LEC)

LEC fit to experiment - NN sector -





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Three-Body Forces

What is the origin of three-body forces?

Nucleons are effective degrees of freedom



"The three-body force is a force that does not exist in a two-nucleon system, but appears in a system with three objects or more" A > 3

As an analogy, if we identify nucleons with human beings and forces with emotions, then jealousy is a good example of a three-body force



From N. Kalantar, FM50

• The first 3N force was introduced by Fujita and Miyazawa in 1957

 In chiral effective theory there are 3 terms (at N²LO) with only two new low energy constants



Goal: Calibrate Hamiltonian and then predict other observables

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Structure models: from shell model to ab-initio methods



Ab-initio methods

Let's now use more fundamental interactions and solve the many-body problem



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***RIUMF *Ab-initio*Shell model:** using realistic interactions in shell model



^{RIUMF} "Ab-initio"shell model: using few-body interactions in shell model

Calcium Isotope Chain

J. D. Holt, et.al., J. Phys. G 39, 085111 (2012)

F. Wienholtz, et al., Nature 498, 346 (2013).



With three-body forces one reproduces precise mass data from the traps



Ab-initio methods

- Start from neutrons and protons interacting with realistic forces
- Solve the non-relativistic quantum mechanical problem of A-interacting nucleons

$$H|\psi_i\rangle = E_i|\psi_i\rangle$$
$$H = T + V_{NN}(\Lambda) + V_{3N}(\Lambda) + \dots$$



• Find numerical solutions with no approximations or controllable approximations



 Calculate low-energy observables for A-body nuclei and compare with experiment to test nuclear forces and provide predictions when experiments are hard or not possible



Ab-initio methods

- Monte Carlo Methods, like Green's Function Monte Carlo, Lattice Effective field theory etc. (Carlson, Lovato, Gandolfi, Lee, ...)
- Faddeev and Faddeev-Yakubovsky methods (Deltuva, Lazauskas,...)
- No Core Shell model methods (Vary, Navratil, Qualgioni, Roth, ...)
- Hyperspherical Harmonics expansions (Barnea, Kievsky, Viviani, Marcucci, ...)



 Coupled-cluster theory (Hagen, Papenbrock, Hjorth-Jensen, ...)



- In-medium SRG (Bogner, Hergert, Holt, Schwenk ...)
- Self consistent Green's functions (Barbieri, Soma,)

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Quantum Monte Carlo methods



This method can go up to ¹²C

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A few-body method (bound states and reactions)

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Hyperspherical Harmonics

A basis set, mostly used for A=3,4. Challenge to go up to A=7,8



• Solve the problem in the CM frame

$$[T + V(r)]\psi(\vec{r}) = E\psi(\vec{r})$$

• Use spherical coordinates

$$\vec{r} = (r, \underline{\theta}, \phi)$$

$$\Omega$$

$$\psi(\vec{r}) \sim Y_{\ell m}(\Omega) u_{\ell}(r)$$

$$\longrightarrow T = T_r - \frac{\hat{\ell}^2}{r^2}$$

$$\hat{\ell}^2 Y_{\ell m}(\Omega) = \ell(\ell+1) Y_{\ell m}(\Omega)$$

Solve the radial equation

$$\left[T_r - \frac{\ell(\ell+1)}{r^2} + V(r) - E\right]u_\ell(r) = 0$$

Three-body Nucleus



• Solve the problem in the CM frame

-
$$[T + V(\eta_1, \eta_2)] \psi(\vec{\eta}_1, \vec{\eta}_2) = E \psi(\vec{\eta}_1, \vec{\eta}_2)$$

• Use hyperspherical coordinates

• Solve the hyperradial equation

only for hyper-radial potentials

$$\left[T_{\rho} - \frac{K(K+4)}{\rho^2} + V(\rho) - E\right] R_K(\rho) = 0$$



Hyperspherical Harmonics

A basis set, mostly used for A=3,4. Challenge to go up to A=7,8



• Solve the problem in the CM frame

$$[T + V(r)]\psi(\vec{r}) = E\psi(\vec{r})$$

• Use spherical coordinates

$$\vec{r} = (r, \underline{\theta}, \phi)$$

$$\Omega$$

$$\psi(\vec{r}) \sim Y_{\ell m}(\Omega) u_{\ell}(r)$$

$$\longrightarrow T = T_r - \frac{\hat{\ell}^2}{r^2}$$

$$\hat{\ell}^2 Y_{\ell m}(\Omega) = \ell(\ell+1) Y_{\ell m}(\Omega)$$

Solve the radial equation

Three-body Nucleus



• Solve the problem in the CM frame

-
$$[T + V(\eta_1, \eta_2)] \psi(\vec{\eta}_1, \vec{\eta}_2) = E\psi(\vec{\eta}_1, \vec{\eta}_2)$$

• Use hyperspherical coordinates

• Solve the hyperradial equation

general case

$$\left[T_r - \frac{\ell(\ell+1)}{r^2} + V(r) - E\right] u_\ell(r) = 0 \qquad \left[\left(T_\rho - \frac{K(K+4)}{\rho^2} - E\right)\delta_{[K],[K']} + \langle \mathcal{Y}_{[K]}|V(\rho,\Omega)|\mathcal{Y}_{[K']}\rangle\right] R_K(\rho) = 0$$

$$\sum_{\nu} e^{-\rho}L_\nu(\rho) \checkmark$$

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Hyperspherical Harmonics

A basis set, mostly used for A=3,4. Challenge to go up to A=7,8





Exact method



Bad computational scaling



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• Exotic nuclei with an interesting structure



 Neutron halos: Large n/p ratio (neutron-rich)

Halo	n/p
⁶ He	2
⁸ He	3
¹¹ Li	2.66
¹² C	1

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 208 Pb



The Helium Isotope Chain



Borromean Nucleus

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Named after Borromean rings by M.V. Zhukov et al., Phys. Rep 231, 151 (1993)



Isola Bella, Lago Maggiore, Italia



pic credit P.Capel

July 7th 2015



Let's solve it as a six-body problem with hyperspherical harmonics expansions



High-precision Penning trap and laser spectroscopy techniques allow accurate measurements of **energies and charge radii** of exotic halo nuclei

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Separation energies from TITAN, Penning trap @ TRIUMF

M. Brodeur *et al.*, PRL **108**, 052504 (2012) S.B. *et al.*, PRC **86**, 034321 (2012)



Need to add three-nucleon forces

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Extension to electroweak reactions

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The Continuum Problem



Lorentz Integral Transform Method

Efros, et al., JPG.: Nucl.Part.Phys. 34 (2007) R459

Reduce the continuum problem to a bound-state problem

$$R(\omega) = \sum_{f} \left| \left\langle \psi_{f} \left| J^{\mu} \right| \psi_{0} \right\rangle \right|^{2} \delta(E_{f} - E_{0} - \omega)$$

$$L(\sigma,\Gamma) = \int d\omega \frac{R(\omega)}{(\omega-\sigma)^2 + \Gamma^2} = \left\langle \tilde{\psi} | \tilde{\psi} \right\rangle < \infty$$



where $\left| \tilde{\psi} \right\rangle$ is obtained solving

$$(H - E_0 - \boldsymbol{\sigma} + i\boldsymbol{\Gamma})|\tilde{\Psi}\rangle = J^{\mu}|\Psi_0\rangle$$

- Due to imaginary part Γ the solution $|\psi
 angle$ is unique
- Since $\langle \tilde{\psi} | \tilde{\psi}
 angle$ is finite, $| \tilde{\psi}
 angle$ has bound state asymptotic behaviour

Use bound-states techniques to solve the Schrödinger equation

$$L(\sigma,\Gamma) \xrightarrow{\text{inversion}} R(\omega)$$

The exact final state interaction is included in the continuum rigorously!



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Giant Dipole Resonance in A=6

with Hyperspherical Harmonics





A many-body method (bound states and reactions)

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Extension to medium-mass nuclei

Develop new many-body methods that can extend the frontiers to heavier and neutron nuclei



• CC is optimal for closed shell nuclei $(1,\pm 2)\pm$

Uses particle coordinates



Coupled-cluster theory

Compared to other methods on the Oxygen isotope chain

Hebeler, Holt, Menendez, Schwenk, Ann. Rev. Nucl. Part. Sci. (2015)



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Coupled-cluster theory

Pushing the limits in mass number ...



S.Binder et al., Physics Letters B 736 (2014) 119-123

But what about reactions?

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Electromagnetic Reactions

Photo-nuclear Reactions

Reactions resulting from the interaction of a photon with the nucleus

For photon energy 15-25 MeV stable nuclei across the periodic table show wide and large peak



Coulomb excitations

Inelastic scattering between two charged particles. Can use unstable nuclei as projectiles.

Neutron-rich nuclei show fragmented low-lying strength



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Electromagnetic Reactions

Photo-nuclear Reactions

Reactions resulting from the interaction of a photon with the nucleus

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LIT with Coupled Cluster Theory

S.B. et al., PRL 111, 122502 (2013)

Present implementation in the CCSD scheme $T=T_1+T_2$ $\hat{R}=\hat{R}_0+\hat{R}_1+\hat{R}_2$

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LIT with Coupled Cluster Theory

Validation for ⁴He

Comparison of CCSD with exact hyperspherical harmonics (HH) with NN forces at N³LO



The comparison with exact theory is very good! Small difference due to missing triples and quadrupoles



LIT with Coupled Cluster Theory

New theoretical method aimed at extending ab-initio calculations towards medium mass

Extension to Dipole Response Function to ¹⁶O/⁴⁰Ca with NN forces derived from χ EFT (N³LO)



First time description of GDR for these nuclei

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Pigmy Resonances in Nuclei

Observed e.g. in coulomb excitation reactions





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Structure models: from shell model to ab-initio methods

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Pigmy Resonances in Nuclei

Other resonances in exotic nuclei which await a microscopic explanation ...



Kanungo et al., Phys. Rev. Lett. 114, 192502 (2015)

Long sought for isoscalar dipole resonance has been observed

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Ab-initio Theory with external probes



N.B.: Two-body currents replace the old shell model language of "effective charges" or "quenching factors"

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Beta Decays



Why is the ¹⁴C half life so anomalously long? 5730ys

$$T_{1/2} = \frac{1}{f(Z, E_0)} \frac{2\pi^3 \hbar^7 \ln 2}{m_e^5 c^4 G_V^2} \frac{1}{g_A^2 |E_A^1|^2}$$

Axial dipole from one- and two-body operators

Maris *et al.*, Phys. Rev. Lett. **106**, 202502 (2011)



3NF needed to explain the long half life of ¹⁴C

Three-body forces and two-body operators are deeply connected



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Beta Decays





Magnetic Moments



Two-body currents have a large effect in exotic nuclei

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Neutrino long baseline experiments (T2K, Miniboon, LBNE, etc.) require theoretical input to simulate the interaction of neutrinos with the detector material (¹²C, ¹⁶O)



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Structure models: from shell model to ab-initio methods



Reactions for Astrophysics



Solar conditions cannot be reproduced in the Lab

Reaction cross sections are measured at higher energy than needed

Need a reliable ab-initio theory (NCSM/RGM) because extrapolations are dangerous

Synergy between experiment and predictive theory is essential

Solar neutrinos measured by SNO and Super-Kamiokande

The predicted solar neutrino flux from the ⁸B decay is proportional to the thermal average rate of the $^{7}\text{Be}(p,\gamma)^{8}\text{B}$ radiative capture reaction



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Structure models: from she



Exciting era in ab-initio nuclear theory with advances on many fronts

The ab-initio approach allows to assess solid theoretical error bars and develop the strong predictive power necessary to tackle exotic nuclei

A strong connection of theory with experiment is fundamental in the physics of radioactive ion beams





Back-up slides

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Structure models: from shell model to ab-initio methods

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Nuclear shell model

Calculate the degeneracy in the nuclear shell model

Case of the spherical HO potential

 $N=2(n-1)+\ell$ defines the shell n-1 number of nodes in $R_{n\ell}(r)$

For fixed N, the angular momentum can vary because n can vary

$$\ell = N - 2(n-1) \implies \ell = N, N - 2, \dots, 2, 0.$$

Because the energy does not depend on the projection m, for a given N, and ℓ we have a degeneracy

$$\begin{array}{ccc} d_N=2 & (2\ell+1) \\ \uparrow & & \\ \text{two possible projections} & \text{all possible values of m for a given } \ell \\ \text{of spin +1/2 or -1/2} \end{array}$$

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Nuclear shell model

Recap of spin-orbit splitting

Spin-orbit splitting

We have to couple the angular momenta also in the wave functions:

$$\varphi_{n\ell jm}(\vec{r}) = R_{n\ell}(r) \ [Y_{\ell}(\hat{r}) \otimes \chi_{1/2}(\sigma)]_m^j$$

To calculate the single particle energy with the new hamiltonian we have to work out the spin-orbit operator

$$\begin{aligned} j^2 &= \vec{j} \cdot \vec{j} = (\vec{\ell} + \vec{s}) \cdot (\vec{\ell} + \vec{s}) = \ell^2 + s^2 + 2\vec{\ell} \cdot \vec{s} \\ \vec{\ell} \cdot \vec{s} &= \frac{1}{2} (j^2 - \ell^2 - s^2) \end{aligned}$$

So that

$$\vec{\ell} \cdot \vec{s} \,\varphi_{n\ell jm}(\vec{r}\,) = \frac{1}{2} (j(j+1) - \ell(\ell+1) - s(s+1))\varphi_{n\ell jm}(\vec{r}\,)$$

So that, the correction to the single particle energy given by the spin-orbit, leads to the following splitting

$$\langle \vec{\ell} \cdot \vec{s} \rangle_{j=\ell+1/2} - \langle \vec{\ell} \cdot \vec{s} \rangle_{j=\ell-1/2} = \frac{1}{2}(2\ell+1)$$
 bigger with increasing orbital angular momentum

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Lorentz Integral Transform Method

Derivation of the bound-state-like equation

Efros, et al., JPG.: Nucl.Part.Phys. 34 (2007) R459

Reduce the continuum problem to a bound-state problem

$$R(\omega) = \sum_{f} \left| \left\langle \psi_{f} \left| J^{\mu} \right| \psi_{0} \right\rangle \right|^{2} \delta(E_{f} - E_{0} - \omega)$$

$$L(\sigma,\Gamma) = \int d\omega \frac{R(\omega)}{(\omega-\sigma)^2 + \Gamma^2} = \left\langle \tilde{\psi} \middle| \tilde{\psi} \right\rangle < \infty$$



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Lorentz Integral Transform Method

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Derivation of the bound-state-like equation

Efros, et al., JPG.: Nucl.Part.Phys. 34 (2007) R459

Reduce the continuum problem to a bound-state problem

$$\begin{split} \mathbf{R}(\omega) &= \int_{f} \left| \left\langle \psi_{f} \left| J^{\mu} \right| \psi_{0} \right\rangle \right|^{2} \delta(\mathbf{E}_{f} - \mathbf{E}_{0} - \omega) \\ \mathbf{L}(\sigma, \Gamma) &= \int d\omega \frac{R(\omega)}{(\omega - \sigma)^{2} + \Gamma^{2}} = \left\langle \tilde{\psi} \right| \tilde{\psi} \right\rangle < \infty \\ &= \int_{f} \left\langle \psi_{0} \right| J^{\mu} \frac{1}{\mathbf{E}_{f} - \mathbf{E}_{0} - \sigma - i\Gamma} \left| \psi_{f} \right\rangle \left\langle \psi_{f} \right| \frac{1}{\mathbf{E}_{f} - \mathbf{E}_{0} - \sigma + i\Gamma} J^{\mu} \right| \psi_{0} \right\rangle \\ &= \int_{f} \left\langle \psi_{0} \right| J^{\mu} \frac{1}{H - \mathbf{E}_{0} - \sigma - i\Gamma} \left| \psi_{f} \right\rangle \left\langle \psi_{f} \right| \frac{1}{H - \mathbf{E}_{0} - \sigma + i\Gamma} J^{\mu} \right| \psi_{0} \right\rangle \\ &= \left\langle \psi_{0} \right| J^{\mu} \frac{1}{H - \mathbf{E}_{0} - \sigma - i\Gamma} \left| \frac{1}{H - \mathbf{E}_{0} - \sigma + i\Gamma} J^{\mu} \right| \psi_{0} \right\rangle \\ &= \left\langle \psi_{0} \right| J^{\mu} \frac{1}{H - \mathbf{E}_{0} - \sigma - i\Gamma} \left| \frac{1}{H - \mathbf{E}_{0} - \sigma + i\Gamma} J^{\mu} \right| \psi_{0} \right\rangle \\ &= \left\langle \psi_{0} \right| J^{\mu} \frac{1}{H - \mathbf{E}_{0} - \sigma - i\Gamma} \left| \frac{1}{H - \mathbf{E}_{0} - \sigma + i\Gamma} J^{\mu} \right| \psi_{0} \right\rangle \\ &= \left\langle \psi_{0} \right| J^{\mu} \frac{1}{H - \mathbf{E}_{0} - \sigma - i\Gamma} \left| \frac{1}{H - \mathbf{E}_{0} - \sigma + i\Gamma} J^{\mu} \right| \psi_{0} \right\rangle \\ &= \left\langle \psi_{0} \right| J^{\mu} \frac{1}{H - \mathbf{E}_{0} - \sigma - i\Gamma} \left| \frac{1}{H - \mathbf{E}_{0} - \sigma + i\Gamma} J^{\mu} \right| \psi_{0} \right\rangle \\ &= \left\langle \psi_{0} \right| J^{\mu} \frac{1}{H - \mathbf{E}_{0} - \sigma - i\Gamma} \left| \frac{1}{H - \mathbf{E}_{0} - \sigma + i\Gamma} J^{\mu} \right| \psi_{0} \right\rangle \\ &= \left\langle \psi_{0} \right| J^{\mu} \frac{1}{H - \mathbf{E}_{0} - \sigma - i\Gamma} \left| \frac{1}{H - \mathbf{E}_{0} - \sigma + i\Gamma} J^{\mu} \right| \psi_{0} \right\rangle \\ &= \left\langle \psi_{0} \right| J^{\mu} \frac{1}{H - \mathbf{E}_{0} - \sigma - i\Gamma} \left| \frac{1}{H - \mathbf{E}_{0} - \sigma + i\Gamma} J^{\mu} \right| \psi_{0} \right\rangle \\ &= \left\langle \psi_{0} \right| J^{\mu} \frac{1}{H - \mathbf{E}_{0} - \sigma - i\Gamma} \left| \frac{1}{H - \mathbf{E}_{0} - \sigma + i\Gamma} J^{\mu} \right| \psi_{0} \right\rangle \\ &= \left\langle \psi_{0} \right| J^{\mu} \frac{1}{H - \mathbf{E}_{0} - \sigma - i\Gamma} \left| \frac{1}{H - \mathbf{E}_{0} - \sigma + i\Gamma} J^{\mu} \right| \psi_{0} \right\rangle \\ &= \left\langle \psi_{0} \right| J^{\mu} \frac{1}{H - \mathbf{E}_{0} - \sigma - i\Gamma} \left| \frac{1}{H - \mathbf{E}_{0} - \sigma + i\Gamma} J^{\mu} \right| \psi_{0} \right\rangle \\ &= \left\langle \psi_{0} \right| J^{\mu} \frac{1}{H - \mathbf{E}_{0} - \sigma + i\Gamma} \left| \frac{1}{\Psi} \right| \psi_{0} \right\rangle \\ &= \left\langle \psi_{0} \right| U^{\mu} \frac{1}{H - \mathbf{E}_{0} - \sigma + i\Gamma} \left| \frac{1}{\Psi} \right| \psi_{0} \right\rangle \\ &= \left\langle \psi_{0} \right| U^{\mu} \frac{1}{H - \mathbf{E}_{0} - \sigma + i\Gamma} \left| \frac{1}{\Psi} \right| \psi_{0} \right\rangle \\ &= \left\langle \psi_{0} \right\rangle \\ \\ &= \left\langle \psi_{0} \right| \psi_{0} \right\rangle \\ \\ &= \left\langle \psi_{0} \right| \psi_{0} \right\rangle \\ \\ &= \left\langle \psi_{0} \right\rangle \\ \\ &= \left\langle \psi_{0} \right| \psi_{0} \right\rangle \\ \\ &= \left\langle \psi_{0} \right$$

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Lorentz Integral Transform Method

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Efros, et al., JPG.: Nucl.Part.Phys. 34 (2007) R459

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$$L(\sigma,\Gamma) = \int d\omega \frac{R(\omega)}{(\omega-\sigma)^2 + \Gamma^2} = \left\langle \tilde{\psi} | \tilde{\psi} \right\rangle < \infty$$



where $\left| \tilde{\psi} \right\rangle$ is obtained solving

$$(H - E_0 - \boldsymbol{\sigma} + i\boldsymbol{\Gamma})|\tilde{\Psi}\rangle = J^{\mu}|\Psi_0\rangle$$

- Due to imaginary part Γ the solution $|\psi
 angle$ is unique
- Since $\langle \tilde{\psi} | \tilde{\psi}
 angle$ is finite, $| \tilde{\psi}
 angle$ has bound state asymptotic behaviour

Use bound-states techniques to solve the Schrödinger equation

$$L(\sigma,\Gamma) \xrightarrow{\text{inversion}} R(\omega)$$

The exact final state interaction is included in the continuum rigorously!



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