Covariant density functional theory and nuclear spin-isospin excitations (I)

Haozhao LIANG (梁豪兆)
RIKEN Nishina Center, Japan
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Lecture 1: Covariant density functional theory
- Introduction
- Theory: Density Functional Theory (DFT)
- Theory: Covariant / relativistic scheme
- Application: 3D calculations for covariant DFT

Lecture 2: Nuclear spin-isospin excitations
- Introduction
- Theory: Random Phase Approximation (RPA)
- Application: Spin-isospin resonances and $\beta$ decays
- Application: Unitarity of Cabibbo-Kobayashi-Maskawa matrix
Chart of Nuclei (2014)
~ 3000 nuclei

- stable nuclei
- unstable nuclei observed so far
- drip-lines (limit of existence) (theoretical predictions)
- magic numbers

~ 300 nuclei
~ 2700 nuclei
~ 6000 nuclei

~ 1500 nuclei

http://www.nishina.riken.go.jp/index_e.html
Radioactive isotope beam facilities

- TRIUMF, ISAC I-II
- NSCL (USA), FRIB (2020)
- GANIL (France), SPIRAL2, Phase 2 (2016-18)
- GSI (Germany), FAIR (2018-20)
- ISOLDE, CERN, HIE-ISOLDE (2014)
- EURISOL (Europe), (Planned)
- RISP (Korea), (Funded)
- RIBF RIKEN (Japan), SRC+BigRIPS (2007)

Best in the world
~70 % speed of light!
“Although QCD is the basic theory of strong interactions, other models must take over for a proper description of the low-energy nuclear behavior.”

“The figure indicates some models used and their region of applicability.”

“Note that the regions overlap, we are progressing towards a complete understanding of nuclear structure.”

Proper energy scale & degree of freedom for understanding the proper physics
Density functional theory (DFT) aims at understanding both ground-state and excited-state properties of thousands of nuclei in a consistent and predictive way.
Nuclear many-body problem

Nuclear $N$-particle system

- Time-dependent Schrödinger/Dirac equation (in this talk $\hbar = c = 1$)

\[ i \frac{\partial \Psi(t)}{\partial t} = \hat{H}\Psi(t) \]

- Stationary equation

\[ \hat{H}\Psi(x_1, x_2, \ldots, x_N) = E\Psi(x_1, x_2, \ldots, x_N) \]

where $x_i = (r_i, \sigma_i, \tau_i)$ stands for the spatial, spin, and isospin coordinates.

The problem becomes extremely difficult when $N = 4, 5, 6, \ldots$

- However, the $N$-particle wave function contains a great deal of information which is irrelevant to most of important physical properties.
- It is very advantageous to introduce the density matrices, defined from the many-body wave function by integrating out much of redundant information.
The aim of density functional theory (DFT) is
- to reduce the many-body quantum mechanical problem formulated in terms of \( N \)-particle wave functions \( \Psi \) to the one-particle level with the local density distribution \( \rho(r) \).

**One-body local density** (a function in 3D space, independent of \( N \))

\[
\rho(r) = \sum_{\sigma,\tau} \int |\Psi(x, x_2, \ldots, x_N)|^2 dx_2 \ldots dx_N
\]
- experimental observable
- with transparent physical meaning
- easily visualized

"Can the aim of DFT be justified?"

http://www.nishina.riken.go.jp/index_e.html

- The non-degenerate ground-state energy $E$ of a system of identical spinless fermions is a unique functional of the local density $\rho(r)$.
- This energy functional $E[\rho]$ attains its minimum value when the density has its correct ground-state value.

Figure 1. Creators of density functional theory. Walter Kohn (left, in 1962) and his two postdoctoral fellows, Pierre Hohenberg (middle, in 1965) and Lu Sham (right, undated), produced their theory in 1964 and 1965. (Photographs courtesy of Walter Kohn and the John Simon Guggenheim Memorial Foundation, Pierre Hohenberg, and Lu Sham.)

In proving their theorem, Hohenberg and Kohn considered a collection of an arbitrary number of electrons enclosed in a large box, moving under the influence of an external potential \( v(r) \) and the mutual Coulomb repulsion.

- Hamiltonian with an external field
  \[
  \hat{H}_v = \hat{H} + \hat{V} \quad \text{with} \quad \hat{V} = \int dx \, v(r) \psi^\dagger(x) \psi(x)
  \]

- Schrödinger equation
  \[
  \hat{H}_v \Psi_v(x_1, x_2, \ldots, x_N) = E_v \Psi_v(x_1, x_2, \ldots, x_N)
  \]

- One-body local density
  \[
  \rho(r) = \sum_{\sigma, \tau} \int |\Psi_v(x, x_2, \ldots, x_N)|^2 dx_2 \ldots dx_N
  \]

- Obviously, \( \Psi_v \) and \( \rho(r) \) are functionals of \( v(r) \).

To prove \( v(r) \) is a unique functional of \( \rho(r) \)

Proof of Hohenberg-Kohn theorem (II)

- Assume that another potential $v'(r)$ leads to the ground-state wave function $Ψ_{v'}$, and the energy $E_{v'}$, but gives rise to the same density $ρ'(r) = ρ(r)$.

- According to variational principle

$$E_{v'} = \langle Ψ_{v'} | Ĥ_{v'} | Ψ_{v'} \rangle < \langle Ψ_v | Ĥ_{v'} | Ψ_v \rangle = E_v + \langle Ψ_v | Ĥ' - Ĥ | Ψ_v \rangle$$

i.e.,

$$E_{v'} < E_v + \int dr [v'(r) - v(r)] ρ(r)$$

- Exactly, in the same way, one gets

$$E_v < E_{v'} - \int dr [v'(r) - v(r)] ρ(r)$$

Therefore, $v(r)$ is a unique functional of $ρ(r)$, so are Hamiltonian $Ĥ_v$, wave function $Ψ_v$, and the expectation values of all operators of interest.
Proof of Hohenberg-Kohn theorem (III)

- One can define a universal functional $F[\rho] = \langle \Psi_v | \hat{H} | \Psi_v \rangle$, which is valid for any number of particles $N$ and for any external field $v(r)$.

- One can also define the energy functional

$$E[\rho] = \langle \Psi_v | \hat{H}_v | \Psi_v \rangle = F[\rho] + \int d\mathbf{r} \, v(\mathbf{r})\rho(\mathbf{r})$$

and prove that

$$E[\rho'] = F[\rho'] + \int d\mathbf{r} \, v(\mathbf{r})\rho'(\mathbf{r}) = \langle \Psi_{v'} | \hat{H}_v | \Psi_{v'} \rangle \geq \langle \Psi_v | \hat{H}_v | \Psi_v \rangle = E[\rho]$$

restricted by the normalization condition

$$N[\rho] = \int d\mathbf{r} \, \rho(\mathbf{r}) = N$$

Hohenberg-Kohn theorem

- The non-degenerate ground-state energy $E$ of a system of identical spinless fermions is a unique functional of the local density $\rho(\mathbf{r})$.

- This energy functional $E[\rho]$ attains its minimum value when the density has its correct ground-state value.
**Nucleus is a self-bound system** (without external potential)

- It is somewhat useless to use the ground-state density in the laboratory frame, because $\rho(r) = \frac{N}{V} \to 0$ ($V \to \infty$).

- DFT theorem for the **intrinsic density** (a wave-packet state)

$$|\Psi\rangle = |\Phi\rangle \otimes |\chi\rangle$$

where $\Phi$ indicates the **intrinsic state** and $\chi$ defines the **spurious motion**.

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See, e.g., PTEP

**Density functional approaches to collective phenomena in nuclei: Time-dependent density functional theory for perturbative and non-perturbative nuclear dynamics**

Takashi Nakatsukasa

RIKEN Nishina Center, Wako, Saitama 351-0198, Japan.
Nucleus has profound shell effects

- difficult to be presented in the local density $\rho(r)$

Kohn and Sham provided a practical solution


- to separate the exact kinetic energy density functional into a major part $T[\rho]$ that is known and the rest which is treated as correlation.

- By taking a non-interacting system as a reference system

$$\rho(r) = \sum_{i=1}^{N} |\phi_i(r)|^2 \quad \text{and} \quad T[\rho] = \sum_{i=1}^{N} \langle \phi_i | - \frac{1}{2M} \nabla^2 |\phi_i\rangle$$

Kohn-Sham equation (self-consistent)

$$\left( -\frac{1}{2M} \nabla^2 + v_s(r) \right) \phi_i(r) = \epsilon_i \phi_i(r) \quad \text{with} \quad v_s(r) = v_{\text{ext}}(r) + \frac{\delta E_H[\rho]}{\delta \rho(r)} + \frac{\delta E_{\text{xc}}[\rho]}{\delta \rho(r)}$$
The legacy of DFT

- One could argue that the algorithms implemented in DFT programs reflect a long sequence of approximations and extensions made by many individuals to the original Hartree-Fock method.

- DFT provides both the scientific justification and the basis for understanding the meaning behind these algorithms.

"for his development of the density-functional theory"
Nucleon-nucleon interaction

http://www.particleadventure.org/

Nobel Prize 1949

Bonn meson-exchange model for NN interaction

Table 5
Meson parameters used in the relativistic (energy-independent) momentum space one-boson-exchange potential (OBEPQ)

<table>
<thead>
<tr>
<th>Meson</th>
<th>$g_\sigma^2/4\pi$</th>
<th>$g_\omega^2/4\pi(k^2 = 0)$</th>
<th>$m_\sigma$ [MeV]</th>
<th>$\Lambda_\sigma$ [GeV]</th>
<th>$n_\sigma$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\pi$</td>
<td>14.6</td>
<td>14.27</td>
<td>138.03</td>
<td>1.3</td>
<td>1</td>
</tr>
<tr>
<td>$\rho$</td>
<td>0.81; [6.1]</td>
<td>0.43</td>
<td>769</td>
<td>2.0</td>
<td>2</td>
</tr>
<tr>
<td>$\eta$</td>
<td>5</td>
<td>3.75</td>
<td>548.8</td>
<td>1.5</td>
<td>1</td>
</tr>
<tr>
<td>$\omega$</td>
<td>20; [0.0]</td>
<td>10.6</td>
<td>782.6</td>
<td>1.5</td>
<td>1</td>
</tr>
<tr>
<td>$\delta$</td>
<td>1.1075</td>
<td>0.64</td>
<td>983</td>
<td>2.0</td>
<td>1</td>
</tr>
<tr>
<td>$\sigma$</td>
<td>8.2797 *</td>
<td>7.07</td>
<td>550 *</td>
<td>2.0</td>
<td>1</td>
</tr>
</tbody>
</table>

Bare NN forces cannot be directly used in DFT calculations.

- The Pauli principle prohibits the scattering into states, which are already occupied in the medium.
- The effective force $G$ is much weaker than bare force $V$, but probably not the case for the tensor part.


“Relativistic description for finite nuclei with nucleon-nucleon interactions from lattice QCD”

S.H. Shen (Peking U.) → RIKEN (2015.8 ~ 2016.5)
with scholarships of PKU & RIKEN short-term IPA
Covariant density functional theory (I)

**Effective Lagrangian density**: starting point of CDFT

\[
\mathcal{L} = \bar{\psi} \left[ i \gamma^\mu \partial_\mu - M - g_\sigma \sigma - \gamma^\mu \left( g_\omega \omega_\mu + g_\rho \vec{\pi} \cdot \vec{\rho}_\mu + e \frac{1 - \tau_3}{2} A_\mu \right) - \frac{f_\pi}{m_\pi} \gamma_5 \gamma^\mu \partial_\mu \vec{\pi} \cdot \vec{\pi} \right] \psi \\
+ \frac{1}{2} \partial^\mu \sigma \partial_\mu \sigma - \frac{1}{2} m_\sigma^2 \sigma^2 - \frac{1}{4} \Omega^{\mu\nu} \Omega_{\mu\nu} + \frac{1}{2} m_\omega^2 \omega_\mu \omega^\mu - \frac{1}{4} \vec{R}_{\mu\nu} \cdot \vec{R}^{\mu\nu} + \frac{1}{2} m_\rho^2 \vec{\rho}_\mu \cdot \vec{\rho}_\mu \\
+ \frac{1}{2} \partial_\mu \vec{\pi} \cdot \partial^\mu \vec{\pi} - \frac{1}{2} m_\pi^2 \vec{\pi} \cdot \vec{\pi} - \frac{1}{4} F^{\mu\nu} F_{\mu\nu}
\]

where \( \Omega^{\mu\nu} \equiv \partial^\mu \omega^\nu - \partial^\nu \omega^\mu \), \( \vec{R}^{\mu\nu} \equiv \partial^\mu \vec{\rho}^\nu - \partial^\nu \vec{\rho}^\mu \), \( F^{\mu\nu} \equiv \partial^\mu A^\nu - \partial^\nu A^\mu \)

- **Legendre transformation**

\[
\mathcal{H} = T^{00} = \frac{\partial \mathcal{L}}{\partial \dot{\phi}_i} \dot{\phi}_i - \mathcal{L}
\]

where \( \phi_i \) represent the nucleon, meson, and photon fields.

- The **Lorentz covariance** is taken into account.

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See, e.g.,
Covariant density functional theory (II)

The Hamiltonian density then is obtained as

\[ \mathcal{H} = \mathcal{H}_N + \mathcal{H}_\sigma + \mathcal{H}_\omega + \mathcal{H}_\rho + \mathcal{H}_\pi + \mathcal{H}_A + \mathcal{H}_{\text{int}}. \]

where the contributions from nucleon, meson and photon fields are

\[ \mathcal{H}_N = \bar{\psi} \left[ -i \gamma \cdot \nabla + M \right] \psi, \]
\[ \mathcal{H}_{\text{int.}} = \bar{\psi} \left[ g_\sigma \sigma + g_\omega \gamma^\mu \omega^\mu + g_\rho \gamma^\mu \vec{\rho} \cdot \vec{\rho}^\mu + \frac{f_\pi}{m_\pi} \gamma_5 \gamma^\mu \nabla \vec{\pi} \cdot \vec{\pi} + e \frac{1 - \tau_3}{2} \gamma^\mu A^\mu \right] \psi, \]
\[ \mathcal{H}_\sigma = \frac{1}{2} \dot{\sigma}^2 + \frac{1}{2} \nabla \sigma \cdot \nabla \sigma + \frac{1}{2} m_\sigma^2 \sigma^2, \]
\[ \mathcal{H}_\omega = -\frac{1}{2} \Omega^{0\nu} \dot{\omega}_\nu + \frac{1}{2} \Omega^{i\nu} \partial_i \omega_\nu - \frac{1}{2} m_\omega^2 \omega^\mu \omega^\mu, \]
\[ \mathcal{H}_\rho = -\frac{1}{2} \bar{R}^{0\nu} \dot{\rho}_\nu + \frac{1}{2} \bar{R}^{i\nu} \partial_i \rho_\nu - \frac{1}{2} m_\rho \bar{\rho} \rho^\mu \cdot \rho^\mu, \]
\[ \mathcal{H}_\pi = \frac{1}{2} \dot{\pi}^2 + \frac{1}{2} \nabla \vec{\pi} \cdot \nabla \vec{\pi} + \frac{1}{2} m_\pi^2 \vec{\pi}^2, \]
\[ \mathcal{H}_A = -\frac{1}{2} \bar{F}_{0\nu} \dot{A}_\nu + \frac{1}{2} F^{i\nu} \partial_i A_\nu. \]
Covariant density functional theory (III)

- Trial wave function (Slater determinant: **mean-field approximation**)
  \[ |\Phi_0\rangle = \prod_k c^\dagger_k |0\rangle \]

Energy functional of the system

\[ E[\rho] = \langle \Phi_0 | \mathcal{H} | \Phi_0 \rangle = E_k + E^D_\sigma + E^D_\omega + E^D_\rho + E^D_A + E^E_\sigma + E^E_\omega + E^E_\rho + E^E_\pi + E^E_A \]

“\(D\)” represents the **direct terms** and “\(E\)” represents the **exchange terms**.

“There is no direct term of \(\pi\). Why?”
Hartree approximation (I)

**Relativistic Mean Field (RMF) = relativistic Hartree approximation**

- Energy functional of the system

\[ E_{\text{RMF}}[\rho] = \langle \Phi_0 | \mathcal{H} | \Phi_0 \rangle \]

\[ = \text{Tr}[\beta(-i\gamma \cdot \nabla + M)\rho] \]

\[ + \text{Tr} \left[ \beta \left( g_\sigma \sigma + g_\omega \gamma^\mu \omega^\mu + g_\rho \gamma^\mu \tilde{\tau} \cdot \tilde{\rho}^\mu + e \frac{1 - \tau_3}{2} \gamma^\mu A^\mu \right) \rho \right] \]

\[ + \int dx \left\{ \frac{1}{2} \dot{\sigma}^2 + \frac{1}{2} \nabla \sigma \cdot \nabla \sigma + \frac{1}{2} m_\sigma^2 \dot{\sigma}^2 - \frac{1}{2} \Omega^{0\nu} \omega_\nu + \frac{1}{2} \Omega^{i\nu} \partial_i \omega_\nu - \frac{1}{2} m_\omega^2 \omega_\mu \omega^\mu \right. \]

\[ - \frac{1}{2} \tilde{R}^{0\nu} \cdot \dot{\tilde{\rho}}_\nu + \frac{1}{2} \tilde{R}^{i\nu} \cdot \partial_i \tilde{\rho}_\nu - \frac{1}{2} m_\rho \tilde{\rho}_\mu \cdot \tilde{\rho}^\mu - \frac{1}{2} F^{0\nu} \dot{A}_\nu + \frac{1}{2} F^{i\nu} \partial_i A_\nu \left\} \right. \]

- time reversal symmetry \( \Rightarrow \) only time-like components of \( \omega_\mu, \tilde{\rho}_\mu, A_\mu \)
- no isospin-mix \( \Rightarrow \) only third component of \( \tilde{\tau}, \tilde{\rho}_\mu \)
- stationary states \( \Rightarrow \) only space derivatives of meson fields

The variation principle with respect to $\phi_i^\dagger$ leads to the **Dirac equation**

$$\left[ \alpha \cdot p + V(r) + \beta \left( M + S(r) \right) \right] \phi_i(r) = \epsilon_i \phi_i(r)$$

with $S(r) = g_\sigma \sigma(r)$ and $V(r) = g_\omega \omega(r) + g_\rho \tau_3 \rho(r) + e \frac{1 - \tau_3}{2} A(r)$

The variation principle with respect to $\sigma$, $\omega_0$, $\rho_0^3$, $A_0$ leads to the **Klein-Gordon equations**

$$(-\Delta + m_\sigma^2)\sigma(r) = -g_\sigma \rho_s(r)$$

$$(-\Delta + m_\omega^2)\omega(r) = g_\omega \rho_v(r)$$

$$(-\Delta + m_\rho^2)\rho(r) = g_\rho \rho_3(r)$$

$$-\Delta A_0(r) = e \rho_c(r)$$

with the **local densities**

$$\rho_s(r) = \sum_{i=1}^{A} \bar{\psi}_i(r) \psi_i(r)$$

$$\rho_v(r) = \sum_{i=1}^{A} \phi_i^\dagger(r) \psi_i(r)$$

$$\rho_3(r) = \sum_{i=1}^{A} \phi_i^\dagger(r) \tau_3 \psi_i(r)$$

$$\rho_c(r) = \sum_{p=1}^{Z} \phi_p^\dagger(r) \psi_p(r)$$

To solve the equations in a **self-consistent** (**iterative**) way.
The scalar and vector potentials are both very big in amplitude, but with opposite signs: $S(r) < 0$ and $V(r) > 0$.

This results in a shallow **Fermi sea** and a deep **Dirac sea**, the latter is responsible for the **large spin-orbit coupling**.

\[ V + S \approx 70 \text{ MeV} \]
\[ V - S \approx 700 \text{ MeV} \]
\[ 2m^* \approx 1200 \text{ MeV} \]
\[ 2m \approx 1800 \text{ MeV} \]
Progress in covariant DFT

Books and Reviews on covariant DFT

- .......
What is going on?

From spherical to deformed --- to break all geometric symmetries

Our goals: To study the physics in exotic deformed nuclei

- correct asymptotic behavior
- to break all geometric symmetries
- exotic shapes / exotic excitation modes
- reasonable computational time

Table:

<table>
<thead>
<tr>
<th>( \beta_{\lambda\mu} = 0 )</th>
<th>( \beta_{20} &gt; 0 )</th>
<th>( \beta_{20} &lt; 0 )</th>
<th>( \beta_{40} &gt; 0 )</th>
</tr>
</thead>
<tbody>
<tr>
<td><img src="image1.png" alt="Sphere" /></td>
<td><img src="image2.png" alt="Deformed1" /></td>
<td><img src="image3.png" alt="Deformed2" /></td>
<td><img src="image4.png" alt="Deformed3" /></td>
</tr>
<tr>
<td>( \beta_{22} \neq 0 )</td>
<td>( \beta_{30} \neq 0 )</td>
<td>( \beta_{32} \neq 0 )</td>
<td>( \beta_{20} \gg 0 )</td>
</tr>
<tr>
<td><img src="image5.png" alt="Deformed4" /></td>
<td><img src="image6.png" alt="Deformed5" /></td>
<td><img src="image7.png" alt="Deformed6" /></td>
<td><img src="image8.png" alt="Deformed7" /></td>
</tr>
</tbody>
</table>

**72Ca**

Courtey of S.G. Zhou
What is going on?

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CDFT on 3D mesh: ground states & excitations

3D mesh calculations for covariant density functional theory

Y. Tanimura, K. Hagino, and H. Z. Liang

PHYSICAL REVIEW C 87, 054310 (2013)

Feasibility of the finite-amplitude method in covariant density functional theory

Haozhao Liang, Takashi Nakatsukasa, Zhongming Niu, and Jie Meng
Imaginary time step (ITS) method

\[ \lim_{\tau \to \infty} e^{-\hbar \tau} \left\{ \psi(0) \right\} = \lim_{\tau \to \infty} \sum_i c_i e^{-\epsilon_i \tau} \left\{ \phi_i \right\} \propto \left\{ \phi_1 \right\} \]

  - Schrödinger equations

- To solve Dirac equations in 3D space
  - Challenge I: **Variational collapse**
  - Challenge II: **Fermion doubling**

Zhang, Sagawa, Yoshino, Hagino, Meng, Prog. Theor. Phys. 120, 129 (2008)
ITS for Schrödinger equations

\[ \lim_{\tau \to \infty} e^{-h\tau} \left| \psi^{(0)} \right\rangle = \lim_{\tau \to \infty} \sum_i c_i e^{-\epsilon_i \tau} \left| \phi_i \right\rangle \propto \left| \phi_1 \right\rangle \]

\[ \lim_{\tau \to \infty} \left\{ e^{-h\tau} \left| \psi_i \right\rangle \right\} \]

\[ i = 1, 2, \ldots, A \]

\[ [h, \rho] = 0 \]
ITS for Dirac equations

\[
\{ \alpha \cdot p + \beta [M + S(r)] + V(r) \} \phi(r) = \epsilon \phi(r)
\]

ITS evolution leads to contamination of single-particle states by the Dirac sea.

To avoid variational collapse: maximizing $\frac{1}{h}$ instead of minimizing $h$.


\[
\frac{\langle \psi | h^{-1} | \psi \rangle}{\langle \psi | \psi \rangle} \leq \frac{1}{\epsilon_1}
\]

- $h$ is unbounded, but $1/h$ is bounded.
Inverse Hamiltonian method

\[
\lim_{\tau \to \infty} e^{\tau/(h-w)} \langle \psi(0) \rangle = \lim_{\tau \to \infty} \sum_{i} c_i e^{\tau/(\epsilon_i-w)} \langle \phi_i \rangle \propto \langle \phi_1 \rangle
\]

For a small step \(\Delta\) \(\quad\) Hagino & Tanimura, Phys. Rev. C 82, 057301 (2010)

\[
\begin{align*}
\langle \psi^{(n+1)} \rangle &= e^{\Delta \tau/(h^{(n)}-w)} \langle \psi^{(n)} \rangle \\
&\simeq \left( 1 + \frac{\Delta \tau}{h^{(n)}-w} \right) \langle \psi^{(n)} \rangle = \langle \psi^{(n)} \rangle + \Delta \tau \langle \varphi^{(n)} \rangle
\end{align*}
\]
with

\[
(h^{(n)} - w) \langle \varphi^{(n)} \rangle = \langle \psi^{(n)} \rangle
\]

TO SOLVE \quad KNOWN
Of the form $Ax = b$ can be solved iteratively, e.g., Krylov subspace method.

- do not need the matrix element of $A$
- only need the result of $Ay$ for any given $y$

\[
(h^{(n)} - w) \varphi^{(n)} = \psi^{(n)}
\]

CR=Conjugate Residual, (Bi)CG=(Bi-)Conjugate Gradient, GP=Generalized Product
Dirac Fermion on lattice $\rightarrow$ spurious states with high momentum and low energy

1D Dirac equation in coordinate space

$$(-i\alpha \partial_x + \beta M)\phi(x) = \epsilon\phi(x)$$

e.g.

$$\partial_x \phi(x) \rightarrow \frac{\phi(i+1) - \phi(i-1)}{2a}$$

1D Dirac equation in momentum space

$$\left(\alpha \frac{1}{a} \sin(pa) + \beta M\right)\tilde{\phi}(p) = \epsilon\tilde{\phi}(p)$$

Dispersion relation

$$\epsilon^2 = M^2 + p^2 \quad \rightarrow \quad \epsilon^2 = M^2 + \frac{\sin^2(pa)}{a^2}$$

{Tanimura, Hagino, HZL, Prog. Theor. Exp. Phys. 2015, 073D01 (2015)}
Solutions of 1D Dirac equation

- **Physical** and **spurious** states have the same energy, and mix with each other.
Wilson Fermion: a famous problem in lattice QCD  

\[ H_W = -i \alpha \cdot \nabla + \beta [M + S(r)] + V(r) - aR \beta \Delta \]

- Dispersion relation (1D, no potential)

\[ \epsilon^2 = \frac{\sin^2(pa)}{a^2} + \left[ M + \frac{4R}{a} \sin^2(pa/2) \right]^2 \]
Higher-order Wilson terms: less effect on physical states, stronger effect on spurious states.

Application in self-consistent CDFT

- Potential energy surfaces (PES) of $^{24}\text{Mg}$ and $^{28}\text{Si}$

- PES of $^8\text{Be}$ compared with the results by HO basis expansion

Excitations in 3D CDFT

Computational challenge for the excitations in deformed systems

A promising solution:

The combination CDFT + FAM works well for the spherical systems.
To develop CDFT + FAM for the deformed systems.
The key of **Density Functional Theory** is to reduce the many-body quantum mechanical problem formulated in terms of \( N \)-particle wave functions to the one-particle level with the local density distribution \( \rho(\mathbf{r}) \), which is justified by the **Hohenberg-Kohn theorem** and accessed by the **Kohn-Sham theory**.

The covariant/relativistic version of nuclear DFT is based on the **Yukawa meson-exchange picture**, which takes the **Lorentz covariance** into account.

Nuclear DFT aims at understanding both ground states and excited states of thousands of nuclei in a consistent and predictive way.
Covariant density functional theory and nuclear spin-isospin excitations (II)

Haozhao LIANG (梁豪兆)
RIKEN Nishina Center, Japan
September 1, 2015
Lecture 1: Covariant density functional theory

- Introduction
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- Theory: Covariant / relativistic scheme
- Application: 3D calculations for covariant DFT

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- Introduction
- Theory: Random Phase Approximation (RPA)
- Application: Spin-isospin resonances and $\beta$ decays
- Application: Unitarity of Cabibbo-Kobayashi-Maskawa matrix
Atomic nucleus is a rich system in physics
- quantum system
- many-body system \((A \sim 100, \text{spin} \& \text{isospin d.o.f.})\)
- finite system (surface, skin, halo, …)
- open system (resonance, continuum, decay, …)

Spin and Isospin are essential degrees of freedom in nuclear physics.

Neutron halos

\(R \sim A^{1/3}? \) Not always!
\(^{11}\text{Li}: \) a size as \(^{208}\text{Pb}\)

Tanihata:1985
Spin and Magic numbers

Nuclear single-particle spectrum

- **Strong spin-orbit interaction**
  \[ (n, l, j = l \pm 1/2) \]
  "Nuclear Magic numbers"

- **Pseudospin symmetry**
  near degeneracy between
  \[
  \begin{align*}
  (n - 1, l + 2, j = l + 3/2) \\
  (n, l, j = l + 1/2)
  \end{align*}
  \]


Nobel Prize 1963
Spin and Magic numbers

Nuclear single-particle spectrum

- **Strong spin-orbit interaction**
  \((n, l, j = l \pm 1/2)\)
  
  “Nuclear Magic numbers”

- **Pseudospin symmetry**
  near degeneracy between

---

Nobel Prize 1963

with 58 figures, 10 tables, and 378 references
The building blocks of nucleus are protons and neutrons. *(isospin doublets)*

**Neutron halos**

$^6\text{Li} \quad ^7\text{Li} \quad ^8\text{Li} \quad ^9\text{Li} \quad ^{10}\text{Li}$

$^1\text{Li}$

*Meng et al., Prog. Part. Nucl. Phys. 57, 470 (2006)*
Isospin and Equation of State

The building blocks of nucleus are protons and neutrons. (isospin doublets)

Equation of State: two kinds of Fermions $\rightarrow$ symmetry energy  
(nuclear physics $\times$ astrophysics)

"2.0 Solar mass neutron star" in the Universe

Demorest et al., Nature 467, 1081 (2010)  
Nuclear spin-isospin physics

Nuclear spin-isospin excitations

- $\beta$-decays in nature
- charge-exchange reactions in lab

These excitations are important to understand

“What are the spin and isospin properties of nuclear force and nuclei?” (nuclear physics)

“Where and how does the rapid neutron-capture process (r-process) happen?” (astrophysics)

“Are there only three families of quarks in nature?” (particle physics)

Key exp. @
RIKEN
RCNP
CERN
GSI
MSU
TRIUMF

......
Covariant density functional theory

- **Fundamental:** Kohn-Sham Density Functional Theory
- **Scheme:** Yukawa meson-exchange nuclear interactions

\[
\mathcal{L} = \bar{\psi} \left[ i \gamma^\mu \partial_\mu - M - g_\sigma \sigma - \gamma^\mu \left( g_\omega \omega_\mu + g_\rho \vec{\rho} \cdot \vec{\rho}_\mu + e \frac{1 - \gamma_3}{2} A_\mu \right) - \frac{f_\pi}{m_\pi} \gamma_5 \gamma^\mu \partial_\mu \vec{\pi} \cdot \vec{\pi} \right] \psi \\
+ \frac{1}{2} \partial^\mu \sigma \partial_\mu \sigma - \frac{1}{2} m_\sigma^2 \sigma^2 - \frac{1}{4} \Omega^{\mu\nu} \Omega_{\mu\nu} + \frac{1}{2} m_\omega^2 \omega_\mu \omega^\mu - \frac{1}{4} \vec{R}_{\mu\nu} \cdot \vec{R}^{\mu\nu} + \frac{1}{2} m_\rho^2 \vec{R}_\mu \cdot \vec{R}_\mu \\
+ \frac{1}{2} \partial_\mu \vec{\pi} \cdot \partial^\mu \vec{\pi} - \frac{1}{2} m_\pi^2 \vec{\pi} \cdot \vec{\pi} - \frac{1}{4} F^{\mu\nu} F_{\mu\nu}
\]

Comparing to traditional non-relativistic DFT

- **Effective Lagrangian**
  connections to underlying theories, QCD at low energy

- **Dirac equation**
  consistent treatment of spin d.o.f. & nuclear saturation properties *(3-body effect)*

- **Lorentz covariant symmetry**
  unification of time-even and time-odd components

**Dirac and RPA equations**

- **Energy functional** of the system
  \[ E[\rho] = \langle \Phi_0 | \mathcal{H} | \Phi_0 \rangle = E_k + E^D_\sigma + E^D_\omega + E^D_\rho + E^D_A + E^E_\sigma + E^E_\omega + E^E_\rho + E^E_\pi + E^E_A \]

- **Dirac equations** for the ground-state properties
  \[ \int dr' h(r, r') \psi(r') = \varepsilon \psi(r), \quad \text{with} \quad h^D(r, r') = [\Sigma_T(r) \gamma_5 + \Sigma_0(r) + \beta \Sigma_5(r)] \delta(r - r'), \]
  \[ h^E(r, r') = \begin{pmatrix} Y_G(r, r') & Y_F(r, r') \\ X_G(r, r') & X_F(r, r') \end{pmatrix}. \]

- **RPA equations** for the vibrational excitation properties
  \[ \begin{pmatrix} \mathcal{A} & \mathcal{B} \\ -\mathcal{B} & -\mathcal{A} \end{pmatrix} \begin{pmatrix} X \\ Y \end{pmatrix} = \omega \nu \begin{pmatrix} X \\ Y \end{pmatrix} \]

- \( \delta E/\delta \rho \) \rightarrow equation of motion for nucleons: **Dirac (-Bogoliubov) equations**

- \( \delta^2 E/\delta \rho^2 \) \rightarrow linear response equation: **(Q)RPA equations**
Particle-hole scheme

Schematic picture of collective excitations

HF

\[ \text{RPA = random phase approximation} \]
\[ = 1p1h + \text{ground-state correlation} \]

1p1h

\[ \text{See, e.g.,} \]
\[ \text{Ring \\ Schuck,} \text{ The Nuclear Many-Body Problem} \text{ (Springer, New York, 1980)} \]

2p2h

- $\sigma$-meson
  
  \[ V_\sigma(1, 2) = -\left[ g_\sigma \gamma_0 \right]_1 \left[ g_\sigma \gamma_0 \right]_2 D_\sigma(1, 2) \]

- $\omega$-meson
  
  \[ V_\omega(1, 2) = \left[ g_\omega \gamma_0 \gamma^\mu \right]_1 \left[ g_\omega \gamma_0 \gamma_\mu \right]_2 D_\omega(1, 2) \]

- $\rho$-meson
  
  \[ V_\rho(1, 2) = \left[ g_\rho \gamma_0 \gamma^\mu \gamma^\nu \right]_1 \cdot \left[ g_\rho \gamma_0 \gamma_\mu \gamma_\nu \right]_2 D_\rho(1, 2) \]

- Pseudovector $\pi$-$N$ coupling
  
  \[ V_\pi(1, 2) = -\left[ \frac{f_\pi}{m_\pi} \gamma_0 \gamma_5 \gamma^k \partial_k \right]_1 \cdot \left[ \frac{f_\pi}{m_\pi} \gamma_0 \gamma_5 \gamma^\nu \partial_\nu \right]_2 D_\pi(1, 2) \]

- Zero-range counter-term of $\pi$-meson
  
  \[ V_{\pi0}(1, 2) = g' \left[ \frac{f_\pi}{m_\pi} \gamma_0 \gamma_5 \gamma \right]_1 \cdot \left[ \frac{f_\pi}{m_\pi} \gamma_0 \gamma_5 \gamma \right]_2 \delta(\mathbf{r}_1 - \mathbf{r}_2), \quad g' = 1/3 \]

- For the correct asymptotic behavior, $g'$ is not a parameter, but must be $1/3$. 
Spin-isospin resonances

CDFT+RPA for spin-isospin resonances (with only Hartree terms)


example: Gamow-Teller resonance (GTR) in $^{208}$Pb ($\Delta S = 1$, $\Delta L = 0$, $J^\pi = 1^+$)

One has to add $\pi$ and fit $g'$ ➔ Self-consistency is lost
Gamow-Teller resonances

CDFT+RPA for Gamow-Teller resonances (with both Hartree & Fock terms)

GTR excitation energies can be reproduced in a fully self-consistent way.

GTR energies and strength

- GTR excitation energies in MeV and strength in percentage of the $3(N - Z)$ sum rule within the RHF+RPA framework. Experimental and the RH+RPA results are given for comparison.

<table>
<thead>
<tr>
<th></th>
<th>$^{48}$Ca</th>
<th></th>
<th>$^{90}$Zr</th>
<th></th>
<th>$^{208}$Pb</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>energy</td>
<td>strength</td>
<td>energy</td>
<td>strength</td>
<td>energy</td>
<td>strength</td>
</tr>
<tr>
<td>experiment</td>
<td>~ 10.5</td>
<td></td>
<td>15.6 ± 0.3</td>
<td></td>
<td>19.2 ± 0.2</td>
<td>60-70</td>
</tr>
<tr>
<td>RHF+RPA</td>
<td>PKO1</td>
<td>10.72</td>
<td>69.4</td>
<td></td>
<td>15.80</td>
<td>68.1</td>
</tr>
<tr>
<td></td>
<td>PKO2</td>
<td>10.83</td>
<td>66.7</td>
<td></td>
<td>15.99</td>
<td>66.3</td>
</tr>
<tr>
<td></td>
<td>PKO3</td>
<td>10.42</td>
<td>70.7</td>
<td></td>
<td>15.71</td>
<td>68.9</td>
</tr>
<tr>
<td>RH+RPA</td>
<td>DD-ME1</td>
<td>10.28</td>
<td>72.5</td>
<td></td>
<td>15.81</td>
<td>71.0</td>
</tr>
</tbody>
</table>


- The pion is not included in PKO2.
**Physical mechanisms of GTR**

**With only Hartree terms**
- No contribution from isoscalar $\sigma$ and $\omega$ mesons, because exchange terms are missing.
- $\pi$-meson is dominant in this resonance.
- $g'$ has to be retted to reproduce the experimental data.

**With both Hartree & Fock terms**
- Isoscalar $\sigma$ and $\omega$ mesons play an essential role via the exchange terms.
- $\pi$-meson plays a minor role.
- $g' = 1/3$ is kept for self-consistency.

Spin-dipole resonances

CDFT+RPA for Spin-dipole resonances ($\Delta S = 1$, $\Delta L = 1$, $J^\pi = 0^-, 1^-, 2^-$)

(Exp.) Wakasa et al., PRC 84, 014614 (2011); (Theory) HZL, Zhao, Meng, Phys. Rev. C 85, 064302 (2012)

- a crucial test for the theoretical predictive power
Nuclear $\beta$ decays and $r$-process nucleosynthesis

EURICA:
Key exp. @ RIKEN

$\beta$ decays and $r$-process nucleosynthesis

EURICA project is providing lots of new $\beta$-decay data towards $r$-process path.

http://ribf.riken.jp/EURICA/
Theses (PhD x 5, Master x 1)
Articles (PRL x 7, PLB x 1, PRC x 3)
Nuclear $\beta$-decay rates and $r$-process flow ($Z = 20 \sim 50$ region)

FRDM+QRPA: widely used nuclear input
RHFB+QRPA: our results

Classical $r$-process calculation shows a faster $r$-matter flow at the $N = 82$ region and higher $r$-process abundances of elements with $A \sim 140$.

Cabibbo-Kobayashi-Maskawa matrix

- quark eigenstates of weak interaction ↔ quark mass eigenstates
- unitarity of CKM matrix ↔ test of Standard Model

\[
\begin{pmatrix}
|V_{ud}| & |V_{us}| & |V_{ub}| \\
|V_{cd}| & |V_{cs}| & |V_{cb}| \\
|V_{td}| & |V_{ts}| & |V_{tb}|
\end{pmatrix} = \begin{pmatrix}
0.97425 \pm 0.00022 & 0.2252 \pm 0.0009 & 0.00415 \pm 0.00049 \\
0.230 \pm 0.011 & 1.006 \pm 0.023 & 0.0409 \pm 0.0011 \\
0.0084 \pm 0.0006 & 0.0429 \pm 0.0026 & 0.89 \pm 0.07
\end{pmatrix}
\]

Nobel Prize 2008

Unitarity test  Particle Data Group 2014

- the most precise test comes form \(|V_{ud}|^2 + |V_{us}|^2 + |V_{ub}|^2\)
- the most precise \(|V_{ud}|\) comes from nuclear \(0^+ \rightarrow 0^+\) superallowed \(\beta\) transitions

Nuclear superallowed \(\beta\) transitions

- experimental measurements
- theoretical corrections (isospin symmetry-breaking corrections)

"Only three families of quarks in nature?"
**Isospin symmetry-breaking corrections $\delta_c$.** All values are expressed in %.

<table>
<thead>
<tr>
<th></th>
<th>PKO1</th>
<th>PKO2</th>
<th>PKO3</th>
<th>DD-ME1</th>
<th>DD-ME2</th>
<th>NL3</th>
<th>TM1</th>
</tr>
</thead>
<tbody>
<tr>
<td>$^{10}$C → $^{10}$B</td>
<td>0.082</td>
<td>0.083</td>
<td>0.088</td>
<td>0.149</td>
<td>0.150</td>
<td>0.124</td>
<td>0.133</td>
</tr>
<tr>
<td>$^{14}$O → $^{14}$N</td>
<td>0.114</td>
<td>0.134</td>
<td>0.110</td>
<td>0.189</td>
<td>0.197</td>
<td>0.181</td>
<td>0.159</td>
</tr>
<tr>
<td>$^{18}$Ne → $^{18}$F</td>
<td>0.270</td>
<td>0.277</td>
<td>0.288</td>
<td>0.424</td>
<td>0.430</td>
<td>0.344</td>
<td>0.373</td>
</tr>
<tr>
<td>$^{26}$Si → $^{26}$Al</td>
<td>0.176</td>
<td>0.176</td>
<td>0.184</td>
<td>0.252</td>
<td>0.252</td>
<td>0.213</td>
<td>0.226</td>
</tr>
<tr>
<td>$^{30}$S → $^{30}$P</td>
<td>0.497</td>
<td>0.550</td>
<td>0.507</td>
<td>0.612</td>
<td>0.633</td>
<td>0.551</td>
<td>0.648</td>
</tr>
<tr>
<td>$^{34}$Ar → $^{34}$Cl</td>
<td>0.268</td>
<td>0.281</td>
<td>0.267</td>
<td>0.368</td>
<td>0.376</td>
<td>0.438</td>
<td>0.320</td>
</tr>
<tr>
<td>$^{38}$Ca → $^{38}$K</td>
<td>0.313</td>
<td>0.330</td>
<td>0.313</td>
<td>0.431</td>
<td>0.441</td>
<td>0.390</td>
<td>0.572</td>
</tr>
<tr>
<td>$^{42}$Ti → $^{42}$Sc</td>
<td>0.384</td>
<td>0.387</td>
<td>0.390</td>
<td>0.515</td>
<td>0.523</td>
<td>0.436</td>
<td>0.443</td>
</tr>
<tr>
<td>$^{26}$Al → $^{26}$Mg</td>
<td>0.139</td>
<td>0.138</td>
<td>0.144</td>
<td>0.198</td>
<td>0.198</td>
<td>0.172</td>
<td>0.179</td>
</tr>
<tr>
<td>$^{34}$Cl → $^{34}$S</td>
<td>0.234</td>
<td>0.242</td>
<td>0.231</td>
<td>0.302</td>
<td>0.307</td>
<td>0.289</td>
<td>0.267</td>
</tr>
<tr>
<td>$^{38}$K → $^{38}$Ar</td>
<td>0.278</td>
<td>0.290</td>
<td>0.276</td>
<td>0.363</td>
<td>0.371</td>
<td>0.334</td>
<td>0.484</td>
</tr>
<tr>
<td>$^{42}$Sc → $^{42}$Ca</td>
<td>0.333</td>
<td>0.334</td>
<td>0.336</td>
<td>0.442</td>
<td>0.448</td>
<td>0.377</td>
<td>0.383</td>
</tr>
<tr>
<td>$^{54}$Co → $^{54}$Fe</td>
<td>0.319</td>
<td>0.317</td>
<td>0.321</td>
<td>0.395</td>
<td>0.393</td>
<td>0.355</td>
<td>0.368</td>
</tr>
<tr>
<td>$^{66}$As → $^{66}$Ge</td>
<td>0.475</td>
<td>0.475</td>
<td>0.469</td>
<td>0.568</td>
<td>0.572</td>
<td>0.560</td>
<td>0.524</td>
</tr>
<tr>
<td>$^{70}$Br → $^{70}$Se</td>
<td>1.140</td>
<td>1.118</td>
<td>1.107</td>
<td>1.232</td>
<td>1.268</td>
<td>1.230</td>
<td>1.226</td>
</tr>
<tr>
<td>$^{74}$Rb → $^{74}$Kr</td>
<td>1.088</td>
<td>1.091</td>
<td>1.071</td>
<td>1.233</td>
<td>1.258</td>
<td>1.191</td>
<td>1.234</td>
</tr>
</tbody>
</table>

HZL, Giai, Meng, PRC 79, 064316 (2009)
## Effect of Coulomb exchange mean field

**◆ Corrections $\delta_c$ in %.

<table>
<thead>
<tr>
<th></th>
<th>PKO1</th>
<th>PKO1*</th>
<th>DD-ME2</th>
</tr>
</thead>
<tbody>
<tr>
<td>$^{10}$C $\rightarrow$ $^{10}$B</td>
<td>0.082</td>
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<td>0.633</td>
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<td>0.359</td>
<td>0.376</td>
</tr>
<tr>
<td>$^{38}$Ca $\rightarrow$ $^{38}$K</td>
<td>0.313</td>
<td>0.406</td>
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<td>0.298</td>
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<td>1.088</td>
<td>1.230</td>
<td>1.258</td>
</tr>
</tbody>
</table>

- PKO1*: same as PKO1, but switching off **Coulomb exchange** mean field.

- Corrections $\delta_c$ with PKO1* are almost the same as those of RH+RPA approach.

- Corrections $\delta_c$ are sensitive to the proper treatments of the Coulomb field, but not sensitive to specific effective interactions.
Isospin corrections & $V_{ud}$

Isospin corrections for superallowed Fermi $\beta$ decay in self-consistent relativistic random-phase approximation approaches

Haozhao Liang (梁豪兆), Nguyen Van Giai, and Jie Meng (孟杰)

Isospin corrections by self-consistent CDFT

$|V_{ud}|^2 + |V_{us}|^2 + |V_{ub}|^2$: 0.997 ~ 1.000 (the 4th family?)

Summary and Perspectives

Atomic nucleus is a rich system in physics

- quantum system
- many-body system ($A \sim 100$, spin & isospin d.o.f.)
- finite system (surface, skin, halo, …)
- open system (resonance, continuum, decay, …)

In these two lectures

- the foundation of density functional theory
- the key formalism of nuclear DFT in covariant scheme
- the self-consistent and relativistic description of nuclear spin-isospin excitations

To understand both ground states and excited states of thousands of nuclei in a consistent and predictive way:

- to study spin and isospin physics in exotic deformed nuclei
- to provide reliable nuclear inputs for interdisciplinary studies in nuclear astrophysics and particle physics
- …..
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