(Time-dependent) Mean-field approaches to nuclear response and reaction

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Contents

• Finite amplitude method (FAM) for TDHF(B)
  – A feasible alternative approach to (Q)RPA
  – Codes developed so far
    • HF(3D)+FAM (3D coordinate-space rep.)
    • HFBRAD(1D)+FAM (1D radial coordinate rep.)
    • HFBTHO(2D)+FAM (2D HO-basis rep.)

• Pygmy dipole resonances in light to medium-heavy nuclei
  – Shell effects/Magic numbers/Neutron skin

• Glauber calculation of reaction cross section
  – Density input from the mean-field calculation
  – Shell effect similar to the PDR
Time-dependent Hartree-Fock (TDHF)

Time-dependent Hartree-Fock equation

\[
\begin{align*}
&i \frac{\partial}{\partial t} \phi_i(t) = \{h(t) + V_{\text{ext}}(t)\} \phi_i(t) \\
&i \frac{\partial}{\partial t} \rho(t) = [h(t) + V_{\text{ext}}(t), \rho(t)]
\end{align*}
\]

\[
\rho(\vec{r}, t) = \sum_{i=1}^{N} \left| \phi_i(\vec{r}, t) \right|^2
\]

\[
h(t) = h[\rho(t)]
\]
TDHFB for superfluid systems

Time-dependent Hartree-Fock-Bogoliubov equation

\[
i \frac{\partial}{\partial t} \Psi_i(t) = \{H(t) + V_{\text{ext}}(t)\} \Psi_i(t)
\]

\[
i \frac{\partial}{\partial t} R(t) = [H(t) + V_{\text{ext}}(t), R(t)]
\]

\[
\Psi_i = \begin{pmatrix} U_i \\ V_i \end{pmatrix}
\]

\[
H(t) = H[R(t)] = \begin{pmatrix} h & \Delta \\ -\Delta^* & -h^* \end{pmatrix}
\]

\[
R(t) = \sum_i \Psi_i \Psi_i^+ = \begin{pmatrix} \rho(t) & \kappa(t) \\ -\kappa^*(t) & 1 - \rho^*(t) \end{pmatrix}
\]
Small-amplitude limit
(Random-phase approximation)

One-body density operator under a TD external potential

\[ i \frac{\hat{\partial}}{\hat{\partial}t} \rho(t) = [h(t) + V_{\text{ext}}(t), \rho(t)] \]

Assuming that the external potential is weak,

\[ \rho(t) = \rho_0 + \delta \rho(t) \quad h(t) = h_0 + \delta h(t) = h_0 + \frac{\delta h}{\delta \rho} \bigg|_{\rho_0} \cdot \delta \rho(t) \]

\[ i \frac{\hat{\partial}}{\hat{\partial}t} \delta \rho(t) = [h_0, \delta \rho(t)] + [\delta h(t) + V_{\text{ext}}(t), \rho_0] \]

Let us take the external field with a fixed frequency \( \omega \),

\[ V_{\text{ext}}(t) = V_{\text{ext}}(\omega)e^{-i\omega t} + V_{\text{ext}}^{+}(\omega)e^{+i\omega t} \]

The density and residual field also oscillate with \( \omega \),

\[ \delta \rho(t) = \delta \rho(\omega)e^{-i\omega t} + \delta \rho^{+}(\omega)e^{+i\omega t} \]

\[ \delta h(t) = \delta h(\omega)e^{-i\omega t} + \delta h^{+}(\omega)e^{+i\omega t} \]
The linear response (RPA) equation

\[ \omega \delta \rho(\omega) = [h_0, \delta \rho(\omega)] + [\delta h(\omega) + V_{\text{ext}}(\omega), \rho_0] \]

Note that all the quantities, except for \( \rho_0 \) and \( h_0 \), are non-hermitian.

\[ \delta \rho(t) = \sum_{i=1}^{A} \left( |\delta \psi_i(t)\rangle \langle \phi_i| + |\phi_i\rangle \langle \delta \psi_i(t)| \right) \]

This leads to the following equations for \( X \) and \( Y \):

\[ \omega \left| X_i(\omega) \right> = (h_0 - \epsilon_i) \left| X_i(\omega) \right> + \hat{Q} \{ \delta h(\omega) + V_{\text{ext}}(\omega) \} |\phi_i\rangle \]

\[ \omega \langle Y_i(\omega) | = -\langle Y_i(\omega) | (h_0 - \epsilon_i) - \langle \phi_i | \{ \delta h(\omega) + V_{\text{ext}}(\omega) \} \hat{Q} \]

\[ \hat{Q} = \sum_{i=1}^{A} (1 - |\phi_i\rangle \langle \phi_i|) \]

These are nothing but the “RPA linear-response equations”. \( X \) and \( Y \) are called “forward” and “backward” amplitudes.
Matrix formulation

\[ \omega |X_i(\omega)\rangle = \left(h_0 - \varepsilon_i\right)|X_i(\omega)\rangle + \hat{Q}\{\delta h(\omega) + V_{\text{ext}}(\omega)\}|\phi_i\rangle \]

\[ \omega \langle Y_i(\omega)\rangle = -\langle Y_i(\omega)\rangle\left(h_0 - \varepsilon_i\right) - \langle \phi_i\rangle\{\delta h(\omega) + V_{\text{ext}}(\omega)\}\hat{Q} \]

(1) \quad \hat{Q} = 1 - \sum_{i=1}^{A} |\phi_i\rangle\langle\phi_i| \]

If we expand the X and Y in particle orbitals:

\[ |X_i(\omega)\rangle = \sum_{m>A} |\phi_m\rangle X_{mi}(\omega) , \quad |Y_i(\omega)\rangle = \sum_{m>A} |\phi_m\rangle Y^*_{mi}(\omega) \]

Taking overlaps of Eq.(1) with particle orbitals

\[ \left\{ \begin{pmatrix} A & B \\ B^* & A^* \end{pmatrix} - \omega \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \right\} \begin{pmatrix} X_{mi}(\omega) \\ Y_{mi}(\omega) \end{pmatrix} = -\begin{pmatrix} (V_{\text{ext}})_{mi} \\ (V_{\text{ext}})_{im} \end{pmatrix} \]

\[ A_{mi,nj} = (\varepsilon_m - \varepsilon_n)\delta_{mn}\delta_{ij} + \langle \phi_m | \frac{\partial h}{\partial \rho_{nj}} | \rho_0 \rangle |\phi_i\rangle \]

\[ B_{mi,nj} = \langle \phi_m | \frac{\partial h}{\partial \rho_{jn}} | \rho_0 \rangle |\phi_i\rangle \]

In many cases, setting \( V_{\text{ext}} = 0 \) and solve the normal modes of excitations:

→ Diagonalization of the matrix
Small-amplitude approximation
--- Linear response (RPA) equation ---

\[
\begin{pmatrix}
A & B \\
B^* & A^*
\end{pmatrix} - \omega
\begin{pmatrix}
1 & 0 \\
0 & -1
\end{pmatrix}
\begin{pmatrix}
X_{mi}(\omega) \\
Y_{mi}(\omega)
\end{pmatrix} = -\begin{pmatrix}
(V_{\text{ext}})_{mi} \\
(V_{\text{ext}})_{im}
\end{pmatrix}
\]

\[
A_{mi,nj} = (\varepsilon_m - \varepsilon)\delta_{mn}\delta_{ij} + \frac{\partial h}{\partial \rho_{nj}}_{\rho_0} |\phi_i\rangle
\]

\[
B_{mi,nj} = \langle \phi_m | \frac{\partial h}{\partial \rho_{jn}}_{\rho_0} | \phi_i \rangle
\]

- Tedious calculation of residual interactions
- Computationally very demanding, especially for deformed systems.

However, in principle, the self-consistent single-particle Hamiltonian should contain everything. We can avoid explicit calculation of residual interactions.
Residual fields can be estimated by the finite difference method:

$$\delta h(\omega) = \frac{1}{\eta} \left( h[\langle \psi' \rangle, \langle \psi \rangle] - h_0 \right)$$

$$|\psi_i\rangle = |\phi_i\rangle + \eta |X_i(\omega)\rangle, \quad \langle \psi'_i \rangle = \langle \phi_i \rangle + \eta \langle Y_i(\omega) \rangle$$

Starting from initial amplitudes $X^{(0)}$ and $Y^{(0)}$, one can use an iterative method to solve the following linear-response equations.

$$\omega |X_i(\omega)\rangle = (h_0 - \epsilon_i) |X_i(\omega)\rangle + \hat{Q} \{ \delta h(\omega) + V_{\text{ext}}(\omega) \} |\phi_i\rangle$$

$$\omega \langle Y_i(\omega) \rangle = -\langle Y_i(\omega) \rangle (h_0 - \epsilon_i) - \langle \phi_i \rangle \{ \delta h(\omega) + V_{\text{ext}}(\omega) \} \hat{Q}$$

Programming of the RPA code becomes very much trivial, because we only need calculation of the single-particle potential, with different bras and kets.
Step-by-step numerical procedure

1. Set the initial amplitudes $X^{(0)}$ and $Y^{(0)}$

2. Calculate the residual fields $\delta h$ by the FAM formula

$$\delta h(\omega) = \frac{1}{\eta} \left( h \langle \psi^\prime | \psi \rangle - h_0 \right)$$

$$|\psi_i\rangle = |\phi_i\rangle + \eta |X_i(\omega)\rangle, \quad \langle \psi_i^\prime \rangle = \langle \phi_i | + \eta \langle Y_i(\omega) |$$

3. Now, we can calculate the l.h.s. of the following equations:

$$\left\{ \begin{align*}
(\omega - h_0 + \varepsilon_i) |X_i(\omega)\rangle - \delta h(\omega) |\phi_i\rangle &= V_{\text{ext}} (\omega) |\phi_i\rangle \\
\langle Y_i(\omega) | (\omega + h_0 - \varepsilon_i) + \langle \phi_i | \delta h(\omega) &= -\langle \phi_i | V_{\text{ext}} (\omega) \\
\end{align*} \right. \Rightarrow A\bar{x} = \bar{b}$$

$$\bar{x} = \begin{pmatrix} |X_i(\omega)\rangle \\ \langle Y_i(\omega) | \end{pmatrix}, \quad \bar{b} = \begin{pmatrix} V_{\text{ext}} (\omega) |\phi_i\rangle \\ -\langle \phi_i | V_{\text{ext}} (\omega) \end{pmatrix}$$

4. Update the amplitude to $(X^{(1)}, Y^{(1)})$ by an iterative algorithm, such as the conjugate gradient method and its derivatives
TDHFB for superfluid systems

Time-dependent Hartree-Fock-Bogoliubov equation

\[ i \frac{\partial}{\partial t} \Psi_i(t) = \{H(t) + V_{\text{ext}}(t)\} \Psi_i(t) \]

\[ i \frac{\partial}{\partial t} R(t) = [H(t) + V_{\text{ext}}(t), R(t)] \]

\[
\Psi_i = \begin{pmatrix} U_i \\ V_i \end{pmatrix} \quad \quad H(t) = H[R(t)] = \begin{pmatrix} h & \Delta \\ -\Delta^* & -h^* \end{pmatrix}
\]

\[
R(t) = \sum_i \Psi_i \Psi_i^* = \begin{pmatrix} \rho(t) & \kappa(t) \\ -\kappa^*(t) & 1 - \rho^*(t) \end{pmatrix}
\]
Residual fields can be calculated by

\[
\delta h(\omega) = \frac{1}{\eta} \left\{ h[\bar{V}_\eta^*, V_\eta] - h_0 \right\}
\]

\[
\delta \Delta(\omega) = \frac{1}{\eta} \left\{ \Delta[\bar{V}_\eta^*, U_\eta] - \Delta_0 \right\}
\]

QRPA equations are

\[
(E_\mu + E_\nu - \omega) X_{\mu\nu} + \delta H_{\mu\nu}^{20} = F_{\mu\nu}^{20}
\]

\[
(E_\mu + E_\nu + \omega) Y_{\mu\nu} + \delta \tilde{H}_{\mu\nu}^{02*} = F_{\mu\nu}^{02}
\]

\[
\begin{pmatrix}
\delta H_{\mu\nu} \\
\delta H_{\mu\nu}^{\tilde{\mu}\tilde{\nu}}
\end{pmatrix}
= W^+ \begin{pmatrix}
\delta h & \delta \Delta \\
\tilde{\delta} \Delta^* & -\delta \tilde{\delta}^*
\end{pmatrix} W
\]

\[
W = \begin{pmatrix}
U & V^* \\
V & U^*
\end{pmatrix}
\]
Implementation of the Finite amplitude method

- (TD)HF (3D coord.) + FAM
  - Implementation by Tsunenori Inakura
  - Inakura, T.N., Yabana, PRC 80, 044301 (2009); arXiv:1106.3618

- Spherical HFB (radial coord.) + FAM
  - Implementation to HFBRAD by Paolo Avogadro
  - Time-odd fields are added
  - Avogadro and T.N., PRC 84, 014314 (2011)

- Deformed HFB + FAM
  - Implementation to HFBTHO by Mario & Markus
  - Time-odd fields are added
  - Stoitsov et al, arXiv:1107.3530
HFBRAD+FAM

Test calculation: IS monopole

Our result: Red line

qp cut-off at 60 MeV

All 2qp states are included.

Calculation by Terasaki et al. (PRC71, 034310 (2005): Green line

<table>
<thead>
<tr>
<th>$^{174}$Sn, $0^+$</th>
<th>$\omega = 4$ MeV</th>
<th>$\omega = 12$ MeV</th>
<th>$\omega = 20$ MeV</th>
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<tbody>
<tr>
<td>$\eta$</td>
<td>$\epsilon$</td>
<td>$N_{\text{iter}}$</td>
<td>$\epsilon$</td>
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<tr>
<td>$10^{-2}$</td>
<td>0.44</td>
<td>1000</td>
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<td>$&lt;10^{-5}$</td>
</tr>
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<td>$10^{-10}$</td>
<td>$&lt;10^{-5}$</td>
<td>161</td>
<td>1.19$\cdot$10$^{-5}$</td>
</tr>
</tbody>
</table>

Linearization parameter

$\eta = 10^{-9} \sim 10^{-5}$
HFBTHO+FAM

- $N_{\text{shell}} = 5$
  - Comparison with Losa et al. PRC 81 (2010) 064307

- $N_{\text{shell}} = 20$
  - Required memory sizes

<table>
<thead>
<tr>
<th>$\nu_{\text{crit}}$</th>
<th>Size of $A$, $B$ matrices</th>
<th>Memory (in GB)</th>
<th>Memory (in GB)</th>
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<tbody>
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<td>$^{40}\text{Mg}$</td>
<td>$32039 \times 32039$</td>
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<tr>
<td>$10^{-3}$</td>
<td>$53386 \times 53386$</td>
<td>45.6</td>
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<td>$10^{-4}$</td>
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<td>$189271 \times 189271$</td>
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<td>$211159 \times 211159$</td>
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<tr>
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<td>848.64</td>
<td>0.572</td>
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</table>

$^{24}\text{Mg}$, SLy4

$\Delta_n = 0.666 \text{ MeV}$

$\Delta_p = 0.665 \text{ MeV}$

$\beta = -0.163$
- Cal. with $N_{\text{shell}} = 20$
  - $^{100}\text{Zr}$
  - $^{240}\text{Pu}$ (g.s. & f.i.)
- Calculation was performed on a laptop PC.
Pygmy dipole resonance (PDR)

  - Strong neutron shell effects
  - Correlation with neutron skin thickness
Magic numbers for PDR emergence

- Zn
- Ni
- Fe
- Cr
- Ti
- Ca
- Ar
- Mg
- Si
- S
- N=15
- N=29

(Up to 10 MeV)
Next magic number: N=51

Z=24

Z=28

Z=32
Magic numbers and low-$l$ orbits

- Magic numbers: $N=15, 29, 51, \ldots$
- Importance of weakly bound orbits with $l=0, 1,$ and $2.$
Pygmy dipole resonance (PDR) and neutron skin thickness

- Reinhard and Nazarewicz, PRC 81, 051303 (2010)
  - Ver weak correlation between PDR and neutron skin thickness
PDR strength vs neutron skin thickness

\[ m_1(PDR)/m_1 \text{ (\%)} \]

\[ R_n - R_p \text{ [ fm]} \]

\[ \nu\text{-rich stable} \]

Weak correlation
(consistent with P.-G. & Witek, PRC81)

Universal correlation with skin thickness

- PDR fraction/ΔR_{np} shows a universal rate, but for specific ranges of neutron numbers.
- The rate is about 0.2 /fm.
Reaction cross section in Glauber theory

Reaction cross section:

\[ \sigma_R = \int db \left( 1 - |e^{i\chi(b)}|^2 \right), \]

Phase shift function:

\[ e^{i\chi(b)} = \left\langle \Psi_0 \Theta_0 \right| \prod \prod \left\{ 1 - \Gamma_{NN}(s_i - t_j + b) \right\} \left| \Psi_0 \Theta_0 \right\rangle. \]

Many-body operator, multiple integral

Profile function:

\[ \Gamma_{NN}(b) = \frac{1 - i\alpha}{4\pi\beta} \sigma_{tot}^{NN} \exp \left( -\frac{b^2}{2\beta} \right) \]

Parameters are fitted to reproduce N-N scattering

\( \alpha \): ratio of the real and imaginary part of the N-N scattering

\( \beta \): slope parameter of the N-N elastic differential cross sections. Give a “range” of the interaction.

E < Pion production threshold

\[ \beta = \frac{1 - \alpha^2}{16\pi \sigma_{tot}^{NN}} \]

E > Pion production threshold

\[ \sigma_{el}^{NN} = \frac{1 - \alpha^2}{16\pi \beta^2} \left( \sigma_{tot}^{NN} \right)^2 \]
Practical way to calculate phase-shift function

\[ G(b, \lambda) = \langle \Phi_0 | \prod_{i=1}^{A} [1 - \lambda \Gamma(b - s_i)] | \Phi_0 \rangle \]

Need
\[ \lambda = 1 \]

Cumulant expansion
\[
\ln G(b, \lambda) = \lambda \left[ \frac{\partial}{\partial \lambda} \ln G(b, \lambda) \right]_{\lambda=0} + \frac{1}{2} \lambda^2 \left[ \frac{\partial^2}{\partial \lambda^2} \ln G(b, \lambda) \right]_{\lambda=0} + \ldots,
\]
\[
\left[ \frac{\partial}{\partial \lambda} \ln G \right]_{\lambda=0} = -\langle \Phi_0 | \sum_{i=1}^{A} \Gamma(b - s_i) | \Phi_0 \rangle = -\int dr \rho(r) \Gamma(b - s)
\]

OLA: Optical Limit Approximation
\[
e^{i \chi_{\text{OLA}}(b)} = \exp \left\{ -\int \int dr dr' \rho_p(r) \rho_T(r') \Gamma_{NN}(s - t + b) \right\}
\]

One-body density distributions are calculated by the 3D HF calculation.
Odd-A nuclei are calculated with the filling approximation.
Ne isotopes at 240AMeV


Mean-field calculation for density provides a reasonable agreement, except for even-odd effects.
Kinks in $\sigma_R$ and in PDR strength are due to s-wave contribution.

Deformation effect is seen in $\sigma_R$. 
Summary

- Finite amplitude method (FAM) provides an alternative feasible approach to linear response calculation.
  - Several codes developed (FAM on 1D-, 2D-HFB, 3D-HF)
  - Systematic analysis on Pygmy Dipole Resonance (PDR)
    - Magic numbers for PDR (N=15, 29, 51, …), which are related to the occupation of low-\(l\) orbitals (s, p, d).
    - Universal correlation between the PDR fraction and the neutron skin thickness; \(m_1(PDR)/m_1 \approx (0.2 / \text{fm}) \Delta R_{np}\).
- Systematic calculations of reaction cross sections for O, Ne, Mg, Si isotopes
  - Qualitative agreement with experimental data
  - The kink at N=14 is consistent with that in PDR fraction
Collaborators

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