Finite amplitude method for TDDFT

Takashi Nakatsukasa (RIKEN Nishina Center)

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Linear response equation

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

$$A_{mi,nj} = (\varepsilon_m - \varepsilon)\delta_{mn}\delta_{ij} + \boxed{\left\langle \phi_m \left| \frac{\partial h}{\partial \rho_{nj}}\right|_{\rho_0} \right| \phi_i \right\rangle}$$

$$B_{mi,nj} = \boxed{\left\langle \phi_m \left| \frac{\partial h}{\partial \rho_{jn}}\right|_{\rho_0} \right| \phi_i \right\rangle}$$

- Tedious calculation of A,B-matrix elements
- Computationally very demanding

$$E\left[\rho_q(t), \tau_q(t), \overleftrightarrow{J}_q(t), \vec{j}_q(t), \vec{s}_q(t), \vec{T}_q(t); \kappa_q(t)\right]$$

kinetic, spin-current, current, spin, spin-kinetic, pair density

However, we can avoid explicit calculation of residual interactions.

Finite amplitude method

T.N., Inakura, Yabana, PRC76 (2007) 024318.

- Linear response (RPA) calculation with a minimum extension of the static DFT code
  - A feasible alternative approach to (Q)RPA
  - Especially useful for a complicated energy functional
  - Codes developed so far in nuclear physics
    - HF(3D)+FAM (3D coordinate-space rep.)
    - HFBRAD(1D)+FAM (1D radial coordinate rep.)
    - HFBTHO(2D)+FAM (2D HO-basis rep.)

Small-amplitude limit (Random-phase approximation)

One-body density operator under a TD external potential

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

Assuming that the external potential is weak,

$$\rho(t) = \rho_0 + \delta\rho(t) \qquad h(t) = h_0 + \delta h(t) = h_0 + \left.\frac{\delta h}{\delta\rho}\right|_{\rho_0} \cdot \delta\rho(t)$$

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

Let us take the external field with a fixed frequency ω,

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

The density and residual field also oscillate with ω,

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

$$\delta h(t) = \delta h(\omega)e^{-i\omega t} + \delta h^{+}(\omega)e^{+i\omega t}$$

The linear response (RPA) equation

$$\omega\delta\rho(\omega) = \left[h_0, \delta\rho(\omega)\right] + \left[\delta h(\omega) + V_{\mathrm{ext}}(\omega), \rho_0\right]$$

Note that all the quantities, except for ρ_0 and h_0, are non-hermitian.

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

$$\Rightarrow \quad \delta\rho(\omega) = \sum_{i=1}^{N}\left(\left|X_i(\omega)\right\rangle\left\langle\phi_i\right| + \left|\phi_i\right\rangle\left\langle Y_i(\omega)\right| \right)$$

This leads to the following equations for X and Y:

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

$$\omega\left\langle Y_i(\omega)\right| = -\left\langle Y_i(\omega)\right|\left(h_0 - \varepsilon_i\right) - \left\langle\phi_i\right|\left\{\delta h(\omega) + V_{\mathrm{ext}}(\omega)\right\}\hat{Q}$$

$$\hat{Q} = 1 - \sum_{i=1}^{N}\left|\phi_i\right\rangle\left\langle\phi_i\right|$$

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

Matrix formulation

$$\omega \left| X_i(\omega) \right\rangle = \left(h_0 - \varepsilon_i \right) \left| X_i(\omega) \right\rangle + \hat{Q} \left\{ \delta h(\omega) + V_{\rm ext}(\omega) \right\} \left| \phi_i \right\rangle$$
$$\omega \left\langle Y_i(\omega) \right| = -\left\langle Y_i(\omega) \right| \left(h_0 - \varepsilon_i \right) - \left\langle \phi_i \right| \left\{ \delta h(\omega) + V_{\rm ext}(\omega) \right\} \hat{Q} \qquad (1)$$

$$\hat{Q} = 1 - \sum_{i=1}^{N} \left| \phi_i \right\rangle \left\langle \phi_i \right|$$

If we expand the X and Y in *particle orbitals*:

$$\left| X_i(\omega) \right\rangle = \sum_{m:\rm unocc} \left| \phi_m \right\rangle X_{mi}(\omega), \quad \left| Y_i(\omega) \right\rangle = \sum_{m:\rm unocc} \left| \phi_m \right\rangle Y_{mi}^*(\omega)$$

Taking overlaps of Eq.(1) with particle orbitals

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

$$A_{mi,nj} = (\varepsilon_m - \varepsilon)\delta_{mn}\delta_{ij} + \left\langle \phi_m \right| \left. \frac{\partial h}{\partial \rho_{nj}} \right|_{\rho_0} \left| \phi_i \right\rangle$$

$$B_{mi,nj} = \left\langle \phi_m \right| \left. \frac{\partial h}{\partial \rho_{jn}} \right|_{\rho_0} \left| \phi_i \right\rangle$$

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

→ Diagonalization of the matrix

Finite Amplitude Method

T.N., Inakura, Yabana, PRC76 (2007) 024318.

Residual fields can be estimated by the finite difference method:

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

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

$$\rho_0 + \delta\rho(\omega) = \sum_i |\psi_i\rangle\langle\psi_i'| = \left(|\phi_i\rangle + \eta|X_i(\omega)\rangle\right)\left(\langle\phi_i| + \eta\langle Y_i(\omega)|\right)$$

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

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

$$\omega\langle Y_i(\omega)| = -\langle Y_i(\omega)|(h_0 - \varepsilon_i) - \langle\phi_i|\{\delta h(\omega) + V_{\mathrm{ext}}(\omega)\}\hat{Q}$$

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 δ h by the FAM formula

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

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

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

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

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

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

For superfluid systems

Kohn-Sham-Bogoliubov equation

$$\boxed{H\Psi_\mu = E_\mu \Psi_\mu}$$

$$\Psi_\mu = \begin{pmatrix} U_\mu \\ V_\mu \end{pmatrix} \qquad H = H[R] = \begin{pmatrix} h[R] - \lambda & \Delta[R] \\ -\Delta^*[R] & -h^*[R] + \lambda \end{pmatrix}$$

$$R(t) = 1 - \sum_i \Psi_i \, \Psi_i^+ = \begin{pmatrix} \rho & \kappa \\ -\kappa^* & 1 - \rho^* \end{pmatrix}$$

In linear response calculation, we need to calculate

$$\delta h = \left.\frac{\delta h}{\delta R}\right|_{R=R_0} \cdot \delta R, \quad \text{and} \quad \delta\Delta = \left.\frac{\delta\Delta}{\delta R}\right|_{R=R_0} \cdot \delta R$$

Finite amplitude method for superfluid systems

Avogadro and TN, PRC **84**, 014314 (2011)

Residual fields can be calculated by

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

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

$$V_\eta = V + \eta U^* Y, \quad \overline{V}_\eta^* = V^* + \eta U X$$

$$U_\eta = U + \eta V^* Y$$

QRPA equations are

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

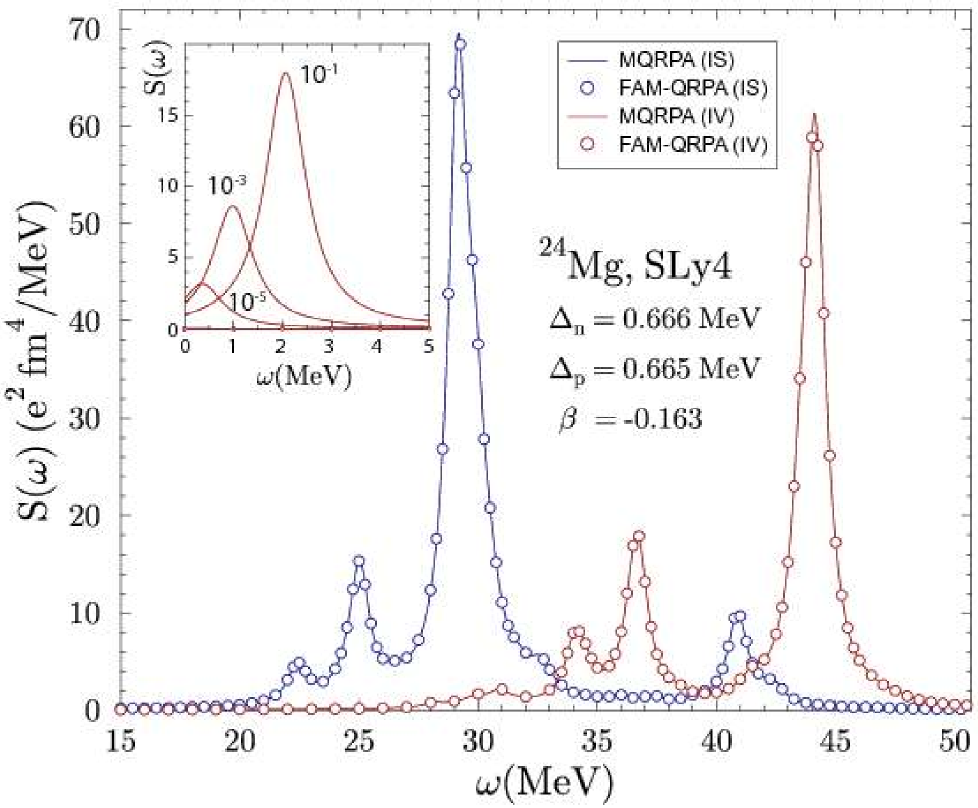
$$(E_\mu + E_\nu + \omega) Y_{\mu\nu} + \delta \widetilde{H}_{\mu\nu}^{02*} = F_{\mu\nu}^{02}$$

$$\begin{pmatrix} & \delta H_{\mu\nu} \\ \delta \widetilde{H}_{\mu\nu} & \end{pmatrix} = W^+ \begin{pmatrix} \delta h & \delta\Delta \\ \delta\widetilde{\Delta}^+ & -\delta h^+ \end{pmatrix} W$$

$$W = \begin{pmatrix} U & V^* \\ V & U^* \end{pmatrix}$$

HFBTHO+FAM

- N_{shell}=5
  - Comparison with Losa et al. PRC 81 (2010) 064307
- N_{shell}=20
  - Required memory sizes



QRPA			FAM
v_{crit}	Size of A, B matrices	Memory (in GB)	Memory (in GB)
^{40}Mg			
10^{-3}	32039×32039	16.4	
10^{-4}	53386×53386	45.6	
10^{-5}	53823×53823	46.35	
10^{-10}	130936×130936	274.31	
10^{-15}	189271×189271	473.18	
10^{-20}	211159×211159	713.41	0.572
^{100}Zr			
10^{-3}	83970×83970	112.81	
10^{-4}	140229×140229	314.63	
10^{-5}	160633×160633	412.85	
10^{-10}	189500×189500	574.56	
10^{-15}	230274×230274	848.41	
10^{-20}	230304×230304	848.64	0.572

Summary

- Finite amplitude method (FAM) provides an alternative feasible approach to linear response calculation.
  - All residual fields can be estimated by the finite difference with respect to the “bra” and “ket”.
  - It can be achieved by a minor extension from the static DFT code
  - Several codes developed (FAM on 1D-, 2D-HFB, 3D-HF) for nuclear physics applications
  - Useful for complicated energy functionals

Collaborators

Paolo Avogadro (RNC/Milano), Shuichiro Ebata (RNC),
Tsunenori Inakura (RNC), Kazuhiro Yabana (Tsukuba/RNC)

Markus Kortelainen (ORNL), Cristina Losa (SISSA),
Witold Nazarewicz (UTK/ORNL), Mario Stoitsov (ORNL)

RNC: RIKEN Nishina Center (Wako, Japan)

ORNL: Oak Ridge Nat. Lab. (Oak Ridge, USA)

UTK: Univ. Tennessee (Knoxville, USA)

SISSA: Scuola Internazionale Superiore di Studi Avanzati (Trieste, Italy)