Applications of time-dependent density-matrix approach

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1) Time-dependent Hartree-Fock theory (TDHF)

Hamiltonian

$$H=\sum_{\lambda\lambda'}\langle\lambda|t|\lambda'\rangle a^{+}_{\lambda}a_{\lambda'}+\frac{1}{2}\sum_{\lambda_1\lambda_2\lambda_1'\lambda_2'}\langle\lambda_1\lambda_2|v|\lambda_1'\lambda_2'\rangle a^{+}_{\lambda_1}a^{+}_{\lambda_2}a_{\lambda_2'}a_{\lambda_1'}$$

Kinetic energy

Effective interaction (Skyrme force)

$\phi_\lambda(\vec{r})$: time independent

TDHF gives time-evolution of 1-body density matrix $n_{\alpha\alpha'}$

$$n_{\alpha\alpha'} = \left\langle \Phi(t) \middle| a^{+}_{\alpha'} a_{\alpha} \middle| \Phi(t) \right\rangle, \qquad \left| \Phi(t) \right\rangle = e^{-iHt/\hbar} \left| \Phi_0 \right\rangle$$

Equation of motion for $n_{\alpha\alpha'}$

$$i\hbar \frac{d}{dt} n_{\alpha\alpha'} = \left\langle \Phi(t) \middle| \left[a^{+}_{\alpha'} a_{\alpha}, H \right] \middle| \Phi(t) \right\rangle$$

$$= \left\langle \Phi(t) \middle| \sum_{\lambda\lambda'} \left\langle \lambda | t | \lambda' \right\rangle (\delta_{\alpha\lambda} a^{+}_{\alpha'} a_{\lambda'} - \delta_{\alpha'\lambda'} a^{+}_{\lambda} a_{\alpha})$$

$$+ \frac{1}{2} \sum_{\lambda_1\lambda_2\lambda_1'\lambda_2'} \left\langle \lambda_1\lambda_2 | v | \lambda_1'\lambda_2' \right\rangle (\delta_{\alpha\lambda_1} a^{+}_{\alpha'} a^{+}_{\lambda_2} a_{\lambda_2'} a_{\lambda_1'} - \delta_{\alpha\lambda_2} a^{+}_{\alpha'} a^{+}_{\lambda_1} a_{\lambda_2'} a_{\lambda_1'}$$

$$- \delta_{\alpha'\lambda_1'} a^{+}_{\lambda_1} a^{+}_{\lambda_2} a_{\lambda_2'} a_{\alpha} + \delta_{\alpha'\lambda_2'} a^{+}_{\lambda_1} a^{+}_{\lambda_2} a_{\lambda_1'} a_{\alpha}) \left| \Phi(t) \right\rangle$$

$$\rho_{\lambda_1'\lambda_2'\alpha'\lambda_2} = \left\langle \Phi(t) \middle| a^+_{\alpha'} a^+_{\lambda_2} a_{\lambda_2'} a_{\lambda_1'} \middle| \Phi(t) \right\rangle \approx n_{\lambda_1'\alpha'} n_{\lambda_2'\lambda_2} - n_{\lambda_1'\lambda_2} n_{\lambda_2'\alpha'}$$

$$\varepsilon_{\alpha\alpha'} = \left\langle \alpha \middle| t \middle| \alpha' \right\rangle + \sum_{\lambda\lambda'} \left\langle \alpha\lambda \middle| v \middle| \alpha'\lambda' \right\rangle_A n_{\lambda'\lambda} = \left\langle \alpha \middle| h \middle| \alpha' \right\rangle$$

$$\Downarrow$$

$$i\hbar \frac{d}{dt} n_{\alpha\alpha'} = \sum_{\lambda} (\varepsilon_{\alpha\lambda} n_{\lambda\alpha'} - \varepsilon_{\lambda\alpha'} n_{\alpha\lambda})$$

TDHF eq. in fixed single-particle basis

$$\begin{pmatrix} \rho(\vec{r}, \vec{r}\,' : t) = \sum_{\alpha\alpha'} n_{\alpha\alpha'} \phi_{\alpha}(\vec{r}) \phi^*_{\alpha'}(\vec{r}\,') \\ i\hbar \frac{d\rho}{dt} = [h, \rho] \end{pmatrix}$$

$$\sum_{\lambda} \rho_{\alpha\lambda\alpha'\lambda} = (N-1) n_{\alpha\alpha'} \approx \sum_{\lambda} (n_{\alpha\alpha'} n_{\lambda\lambda} - n_{\alpha\lambda} n_{\lambda\alpha'}) \Rightarrow n_{\alpha\alpha'} = \sum_{\lambda} n_{\alpha\lambda} n_{\lambda\alpha'}$$

Limitation of Hartree-Fock theory（HF)

HF ground state = a stationary solution of TDHF eq.

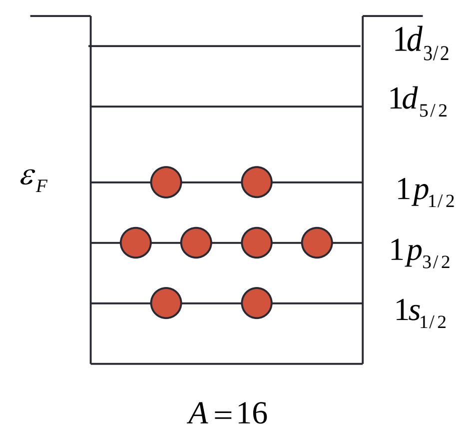
$$i\hbar \frac{d}{dt} n_{\alpha\alpha'} = \sum_{\lambda} (\varepsilon_{\alpha\lambda} n_{\lambda\alpha'} - \varepsilon_{\lambda\alpha'} n_{\alpha\lambda}) = 0$$

$\varepsilon_{\alpha\alpha'}$ and $n_{\alpha\alpha'}$ can be diagonal as $\varepsilon_{\alpha\alpha'} = \delta_{\alpha\alpha'}\varepsilon_{\alpha}$ and $n_{\alpha\alpha'} = \delta_{\alpha\alpha'} n_{\alpha}$ $\quad (h\phi_{\alpha} = \varepsilon_{\alpha}\phi_{\alpha})$

$$n_{\alpha\alpha'} = \sum_{\lambda} n_{\alpha\lambda} n_{\lambda\alpha'} \Rightarrow n_{\alpha} = n_{\alpha} n_{\alpha} \Rightarrow n_{\alpha} = 1 \text{ or } 0$$

$|\Phi_0\rangle$ is a single Slater determinant

$$|\Phi_0\rangle = \prod_{i=1}^{A} a_i^{+} |0\rangle$$



$n_{\lambda} = 0$

$n_{\lambda} = 1$

Occupation probabilities of doubly closed-shell nuclei

Nucleus	j^p	SF(HF)	SF(Exp)(*e*,*e*'*p*)	SF(Exp)/SF(HF)
^{16}O	$1/2^+$	2.00	1.27 ± 0.13	0.64 ± 0.07
^{40}Ca	$3/2^+$	4.00	2.58 ± 0.19	0.65 ± 0.05
^{48}Ca	$1/2^+$	2.00	1.07 ± 0.07	0.54 ± 0.04
^{208}Pb	$1/2^+$	2.00	0.98 ± 0.09	0.49 ± 0.05

$2j+1$

J. Lee et al.,nucl-ex/0511023

$n_\alpha < 1 \longrightarrow$ Ground state is highly correlated.
HF is too simple

Limitation of random phase approximation（RPA)

RPA formulation

- Small amplitude limit of TDHF
- Equation-of-motion approach

Small amplitude limit of TDHF

$$\left|\Psi(t)\right\rangle \approx \left|\Psi_0\right\rangle + \lambda \sum e^{-i\omega_\mu t/\hbar} \left|\Psi_\mu\right\rangle, \qquad \lambda << 1$$

$$i\hbar \frac{d}{dt} n_{\alpha\alpha'} = i\hbar \frac{d}{dt} \left\langle \Psi(t) \right| a^+_{\alpha'} a_\alpha \left| \Psi(t) \right\rangle = \left\langle \Psi(t) \right| [a^+_{\alpha'} a_\alpha, H] \left| \Psi(t) \right\rangle$$

$$\approx \lambda \sum \left(\omega_\mu \left\langle \Psi_0 \right| a^+_{\alpha'} a_\alpha \left| \Psi_\mu \right\rangle e^{-i\omega_\mu t/\hbar} - \omega_\mu \left\langle \Psi_\mu \right| a^+_{\alpha'} a_\alpha \left| \Psi_0 \right\rangle e^{i\omega_\mu t/\hbar} \right)$$

$$= \lambda \sum \left(\left\langle \Psi_0 \right| [a^+_{\alpha'} a_\alpha, H] \left| \Psi_\mu \right\rangle e^{-i\omega_\mu t/\hbar} + \left\langle \Psi_\mu \right| [a^+_{\alpha'} a_\alpha, H] \left| \Psi_0 \right\rangle e^{i\omega_\mu t/\hbar} \right)$$

$$\Downarrow$$

$$\left\langle \Psi_0 \right| [a^+_{\alpha'} a_\alpha, H] \left| \Psi_\mu \right\rangle = \omega_\mu \underline{\left\langle \Psi_0 \right| a^+_{\alpha'} a_\alpha \left| \Psi_\mu \right\rangle} = \omega_\mu \tilde{x}^\mu_{\alpha\alpha'}$$

$\tilde{x}^\mu_{\alpha\alpha'}$: Transition amplitude

$$\left\langle \Psi_0 \middle| [a^+_{\alpha'} a_\alpha, H] \middle| \Psi_\mu \right\rangle \approx (\varepsilon_\alpha - \varepsilon_{\alpha'}) \tilde{x}^\mu_{\alpha\alpha'} + (n_{\alpha'} - n_\alpha) \sum_{\lambda_1 \lambda_1'} \left\langle \alpha\lambda_1 \middle| v \middle| \alpha'\lambda_1' \right\rangle_A \tilde{x}^\mu_{\lambda_1'\lambda_1} = \omega_\mu \tilde{x}^\mu_{\alpha\alpha'}$$

Using $\tilde{x}^\mu_{mi} = x^\mu_{mi}$ and $\tilde{x}^\mu_{im} = -y^\mu_{mi}$, we obtain RPA equations

$$\boxed{\begin{aligned} (\varepsilon_m - \varepsilon_i) x^\mu_{mi} + \sum_{nj} \left\langle mj \middle| v \middle| in \right\rangle_A x^\mu_{nj} + \sum_{nj} \left\langle mn \middle| v \middle| ij \right\rangle_A y^\mu_{nj} = \omega_\mu x^\mu_{mi} \\ (\varepsilon_m - \varepsilon_i) y^\mu_{mi} + \sum_{nj} \left\langle ij \middle| v \middle| mn \right\rangle_A x^\mu_{nj} + \sum_{nj} \left\langle in \middle| v \middle| mj \right\rangle_A y^\mu_{nj} = -\omega_\mu y^\mu_{mi} \end{aligned}}$$

i, j: hole states

m, n: particle states

Matrix form

$$\begin{pmatrix} A & B \\ B^* & A^* \end{pmatrix} \begin{pmatrix} x^\mu \\ y^\mu \end{pmatrix} = \omega_\mu \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} x^\mu \\ y^\mu \end{pmatrix}$$

$$A_{minj} = (\varepsilon_m - \varepsilon_i) \delta_{mn} \delta_{ij} + \left\langle mj \middle| v \middle| in \right\rangle_A$$

$$B_{minj} = \left\langle mn \middle| v \middle| ij \right\rangle_A$$

Equation-of-motion approach

$$Q_\mu^+ = \sum_{mi} x_{mi}^\mu a_m^+ a_i - \sum_{mi} y_{mi}^\mu a_i^+ a_m$$

$$Q_\mu |\Psi_0\rangle = 0, \quad Q_\mu^+ |\Psi_0\rangle = |\Psi_\mu\rangle, \quad H|\Psi_0\rangle = E_0|\Psi_0\rangle, \quad H|\Psi_\mu\rangle = E_\mu|\Psi_\mu\rangle$$

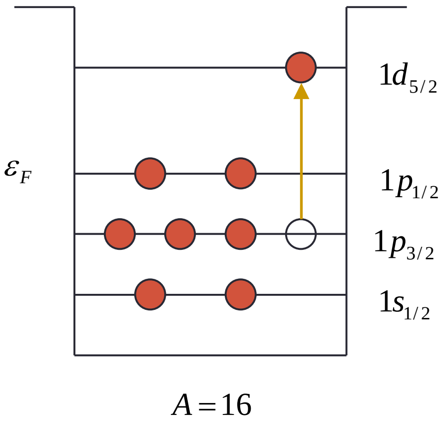
$$\langle\Psi_0|[a_{\alpha'}^+ a_\alpha, H]|\Psi_\mu\rangle = (E_\mu - E_0)\langle\Psi_0|a_{\alpha'}^+ a_\alpha|\Psi_\mu\rangle$$

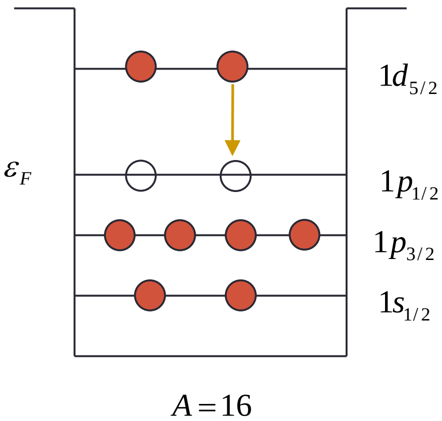
$$\langle\Psi_0|[[a_{\alpha'}^+ a_\alpha, H], Q_\mu^+]|\Psi_0\rangle = \omega_\mu \langle\Psi_0|[a_{\alpha'}^+ a_\alpha, Q_\mu^+]|\Psi_0\rangle$$

$$\downarrow$$

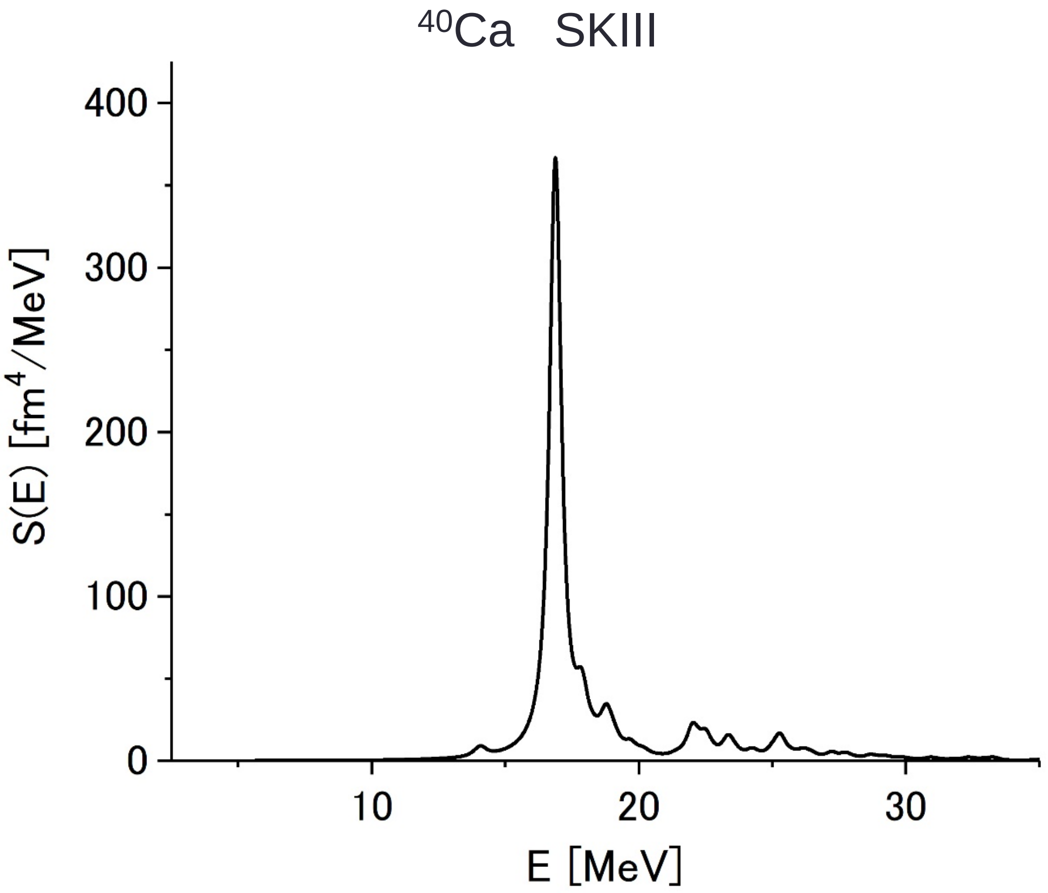
RPA equations

$$\begin{pmatrix} A & B \\ B^* & A^* \end{pmatrix}\begin{pmatrix} x^\mu \\ y^\mu \end{pmatrix} = \omega_\mu \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}\begin{pmatrix} x^\mu \\ y^\mu \end{pmatrix}$$

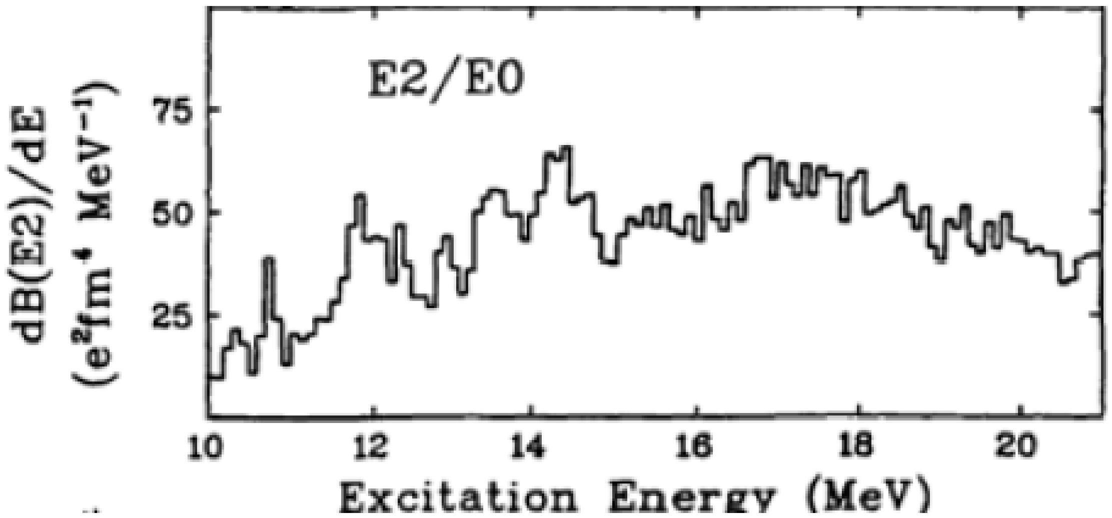




E2 strength distribution in RPA



^{40}Ca(e,$e'x$)



H. Diesner et al. Phys. Rev. Lett. 72, 1994(1994)

Strong fragmentation → RPA is insufficient

2) Time-dependent density-matrix approach (TDDM)

TDDM gives time-evolution of 1-body and 2-body density matrices, $n_{\alpha\alpha'}$ and $C_{\alpha\beta\alpha'\beta'}$

$$n_{\alpha\alpha'} = \langle \Phi(t) | a^{+}_{\alpha'} a_{\alpha} | \Phi(t) \rangle$$

$$C_{\alpha\beta\alpha'\beta'} = \langle \Phi(t) | a^{+}_{\alpha'} a^{+}_{\beta'} a_{\beta} a_{\alpha} | \Phi(t) \rangle - (n_{\alpha\alpha'} n_{\beta\beta'} - n_{\alpha\beta'} n_{\alpha'\beta})$$

$$|\Phi(t)\rangle = e^{-iHt/\hbar} |\Phi_0\rangle$$

Advantages of TDDM

- TDDM is straightforward extension of TDHF
- TDDM gives self-consistent extensions of HF and RPA

Equation for $n_{\alpha\alpha'}$

$$i\hbar\frac{d}{dt}n_{\alpha\alpha'}=\left\langle\Phi(t)\right|\left[a_{\alpha'}^{+}a_{\alpha},H\right]\left|\Phi(t)\right\rangle$$

$$=\left\langle\Phi(t)\right|\sum_{\lambda\lambda'}\left\langle\lambda\left|t\right|\lambda'\right\rangle(\delta_{\alpha\lambda}a_{\alpha'}^{+}a_{\lambda'}-\delta_{\alpha'\lambda'}a_{\lambda}^{+}a_{\alpha})$$

$$+\frac{1}{2}\sum_{\lambda_1\lambda_2\lambda_1'\lambda_2'}\left\langle\lambda_1\lambda_2\left|v\right|\lambda_1'\lambda_2'\right\rangle(\delta_{\alpha\lambda_1}a_{\alpha'}^{+}a_{\lambda_2}^{+}a_{\lambda_2'}a_{\lambda_1'}-\delta_{\alpha\lambda_2}a_{\alpha'}^{+}a_{\lambda_1}^{+}a_{\lambda_2'}a_{\lambda_1'}$$

$$-\delta_{\alpha'\lambda_1'}a_{\lambda_1}^{+}a_{\lambda_2}^{+}a_{\lambda_2'}a_{\alpha}+\delta_{\alpha'\lambda_2'}a_{\lambda_1}^{+}a_{\lambda_2}^{+}a_{\lambda_1'}a_{\alpha})\left|\Phi(t)\right\rangle$$

$$\left\langle \Phi(t) \middle| a^{+}_{\alpha'} a^{+}_{\lambda_2} a_{\lambda_2'} a_{\lambda_1'} \middle| \Phi(t) \right\rangle = n_{\lambda_1'\alpha'} n_{\lambda_2'\lambda_2} - n_{\lambda_1'\lambda_2} n_{\lambda_2'\alpha'} + \underline{C_{\lambda_1'\lambda_2'\alpha'\lambda_2}}$$

$$\Downarrow$$

$$i\hbar \frac{d}{dt} n_{\alpha\alpha'} = \sum_{\lambda} (\varepsilon_{\alpha\lambda} n_{\lambda\alpha'} - \varepsilon_{\lambda\alpha'} n_{\alpha\lambda})$$

$$+ \underline{\sum_{\lambda_2\lambda_1'\lambda_2'} \left\langle \alpha\lambda_2 \middle| v \middle| \lambda_1'\lambda_2' \right\rangle C_{\lambda_1'\lambda_2'\alpha'\lambda_2} - \sum_{\lambda_1\lambda_2\lambda_2'} \left\langle \lambda_1\lambda_2 \middle| v \middle| \alpha'\lambda_2' \right\rangle C_{\alpha\lambda_2'\lambda_1\lambda_2}}$$

For $C_{\alpha\beta\alpha'\beta'} = 0$

$$\Rightarrow i\hbar \frac{d}{dt} n_{\alpha\alpha'} = \sum_{\lambda} (\varepsilon_{\alpha\lambda} n_{\lambda\alpha'} - \varepsilon_{\lambda\alpha'} n_{\alpha\lambda})$$

TDHF equation

Equation for $C_{\alpha\beta\alpha'\beta'}$

$$\boxed{\begin{aligned} i\hbar\frac{d}{dt}C_{\alpha\beta\alpha'\beta'} &= \left\langle \Phi(t) \middle| \left[a_{\alpha'}^{+} a_{\beta'}^{+} a_{\beta} a_{\alpha}, H \right] \middle| \Phi(t) \right\rangle \\ &= (\varepsilon_{\alpha} + \varepsilon_{\beta} - \varepsilon_{\alpha'} - \varepsilon_{\beta'}) C_{\alpha\beta\alpha'\beta'} + B_{\alpha\beta\alpha'\beta'} + P_{\alpha\beta\alpha'\beta'} + H_{\alpha\beta\alpha'\beta'} + T_{\alpha\beta\alpha'\beta'} \end{aligned}}$$

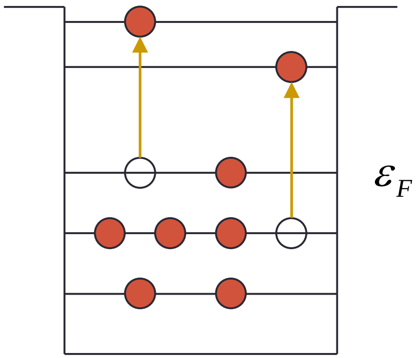
B term: 2 particle – 2 hole excitations

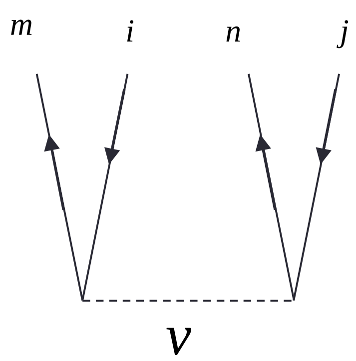
$$B_{\alpha\beta\alpha'\beta'} = \langle \alpha\beta | v | \alpha'\beta' \rangle_A \left[\bar{n}_\alpha \bar{n}_\beta n_{\alpha'} n_{\beta'} - n_\alpha n_\beta \bar{n}_{\alpha'} \bar{n}_{\beta'} \right] \quad , \bar{n}_\alpha = 1 - n_\alpha$$

For $n_{\alpha\alpha'} = n_\alpha \delta_{\alpha\alpha'}, \quad n_\alpha = 0,\ 1$

$$B_{mnij} = \langle mn | v | ij \rangle_A$$

i, j: hole states
m, n: particle states



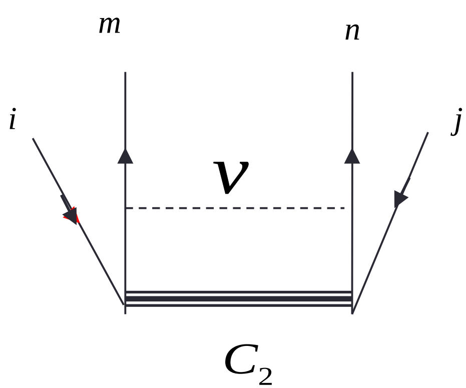


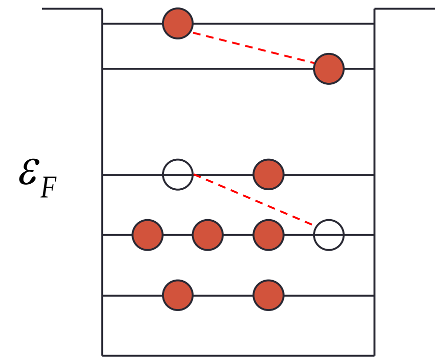
P term: particle – particle and hole – hole correlations

$$P_{\alpha\beta\alpha'\beta'} = \sum_{\lambda\lambda'} \left[\left(1-n_\alpha - n_\beta\right) \langle \alpha\beta | v | \lambda\lambda' \rangle C_{\lambda\lambda'\alpha'\beta'} - C_{\alpha\beta\lambda\lambda'} \langle \lambda\lambda' | v | \alpha'\beta' \rangle \left(1 - n_{\alpha'} - n_{\beta'}\right) \right]$$

For $\quad n_{\alpha\alpha'} = n_\alpha \delta_{\alpha\alpha'}, \quad n_\alpha = 0,\ 1$

$$P_{mnij} = \sum_{m'n'} \langle mn | v | m'n' \rangle\, C_{m'n'ij} + \sum_{i'j'} \langle i'j' | v | ij \rangle\, C_{mni'j'}$$



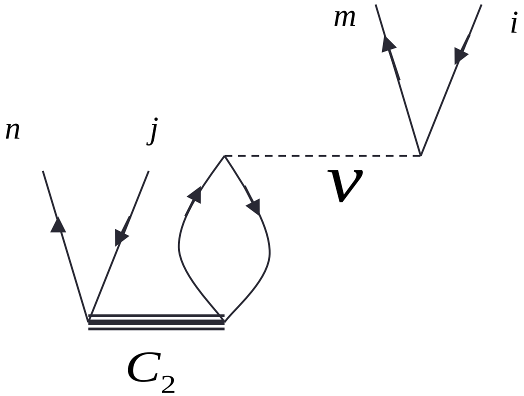


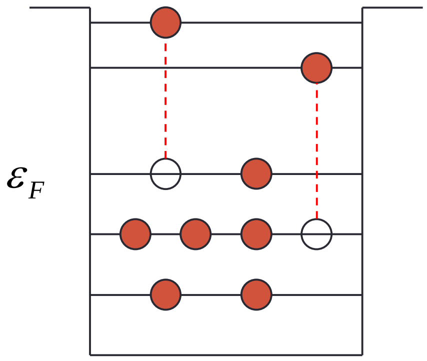
H term: particle – hole correlations

$$H_{\alpha\beta\alpha'\beta'} = \sum_{\lambda\lambda'} (n_{\alpha'} - n_{\alpha}) \langle \alpha\lambda | v | \alpha'\lambda' \rangle_A C_{\lambda'\beta\lambda\beta'} + \{\alpha \leftrightarrow \beta, \alpha' \leftrightarrow \beta'\}$$

For $\quad n_{\alpha\alpha'} = n_{\alpha}\delta_{\alpha\alpha'}, \quad n_{\alpha} = 0,\ 1$

$$H_{mnij} = \sum_{m'i'} [\langle mi'|v|im'\rangle_A C_{m'ni'j} + \langle ni'|v|jm'\rangle_A C_{m'mi'i} - \langle ni'|v|im'\rangle_A C_{m'mi'j} - \langle mi'|v|jm'\rangle_A C_{m'ni'i}]$$





T term： coupling to C_3

$$T_{\alpha\beta\alpha'\beta'} = \sum_{\lambda\lambda'\lambda''} \langle \alpha\lambda | v | \lambda'\lambda'' \rangle C_{\lambda'\lambda''\beta\alpha'\lambda\beta'} + \{\alpha \leftrightarrow \beta, \alpha' \leftrightarrow \beta'\}$$

Equations for $n_{\alpha\alpha'}$ and $C_{\alpha\beta\alpha'\beta'}$

$$i\hbar \frac{dn_{\alpha\alpha'}}{dt} = \left\langle \Phi(t) \middle| [a^+_{\alpha'} a_\alpha, H] \middle| \Phi(t) \right\rangle = F_1(n, C_2)$$

$$i\hbar \frac{dC_{\alpha\beta\alpha'\beta'}}{dt} = \left\langle \Phi(t) \middle| [a^+_{\alpha'} a^+_{\beta'} a_\beta a_\alpha, H] \middle| \Phi(t) \right\rangle = F_2(n, C_2, C_3)$$

$$\vdots$$

Bogoliubov-Born-Green-Kirkwood-Yvon
(BBGKY) hierarchy

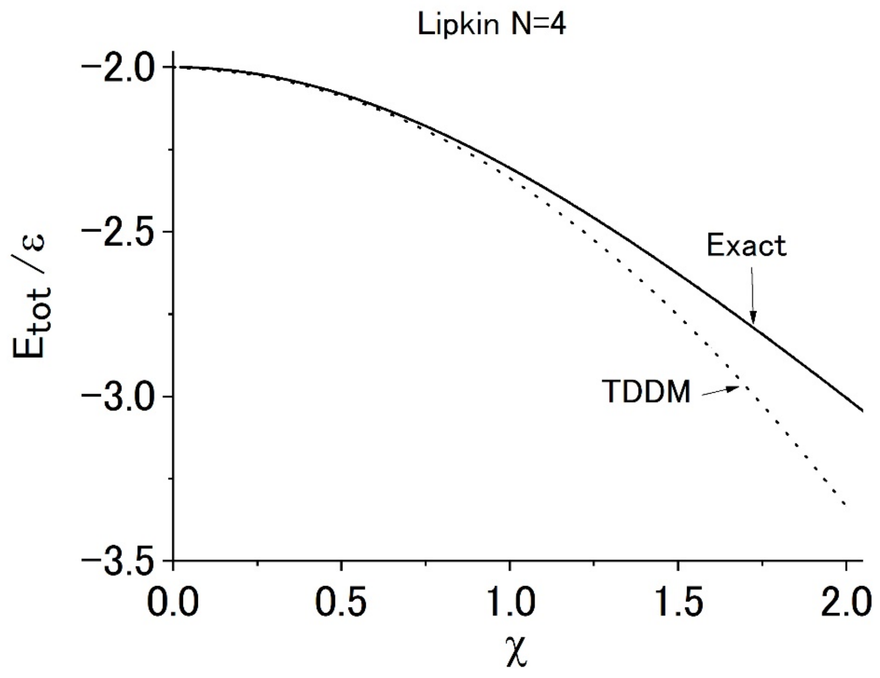
To truncate BBGKY we need to approximate C_3

Truncation schemes of BBGKY hierarchy

- Simplest truncation (TDDM):

$$\boxed{C_3 = 0}$$

(Wang & Cassing, Ann. Phys. 159, 328(1985))



TDDM overestimates
2-body correlations

- TDDM1: (Tohyama & Schuck, Eur. Phys. J. A 50, 7(2014))

$$\boxed{\begin{aligned} C_{p_1p_2h_1p_3p_4h_2} &\approx \sum_h C_{hh_1p_3p_4} C_{p_1p_2h_2h} \\ C_{p_1h_1h_2p_2h_3h_4} &\approx \sum_p C_{h_1h_2p_2p} C_{p_1ph_3h_4} \end{aligned}}$$

Coupled-Cluster-Doubles (CCD)-like ground state

$$\left|Z\right\rangle = e^Z \left|\mathrm{HF}\right\rangle, \quad Z = \frac{1}{4}\sum_{pp'hh'} z_{pp'hh'} a_p^+ a_{p'}^+ a_{h'} a_h$$

gives

$$C_{pp'hh'} \approx z_{pp'hh'}\,,\, C_{hh'pp'} \approx z^*_{pp'hh'}$$

$$C_{p_1p_2h_1p_3p_4h_2} \approx \sum_h z^*_{p_3p_4hh_1} z_{p_1p_2h_2h}\,,\, C_{p_1h_1h_2p_2h_3h_4} \approx \sum_p z^*_{p_2ph_1h_2} z_{p_1ph_3h_4}$$

- TDDM2: Lipkin model with large N

Tohyama & Schuck, Eur. Phys. J. A 53, 186 (2017)

$$\boxed{\begin{aligned} C_{p_1p_2h_1p_3p_4h_2} &\approx \frac{1}{N}\sum_h C_{hh_1p_3p_4}C_{p_1p_2h_2h} \\ C_{p_1h_1h_2p_2h_3h_4} &\approx \frac{1}{N}\sum_p C_{h_1h_2p_2p}C_{p_1ph_3h_4} \end{aligned}}$$

$$N = 1 + \frac{1}{4}\sum_{pp'hh'} C_{pp'hh'}C^*_{pp'hh'}$$

Ground-state calculation

Ground state = a stationary solution of TDDM equations

$$i\hbar\frac{dn_{\alpha\alpha'}}{dt}=0,\quad i\hbar\frac{dC_{\alpha\beta\alpha'\beta'}}{dt}=0$$

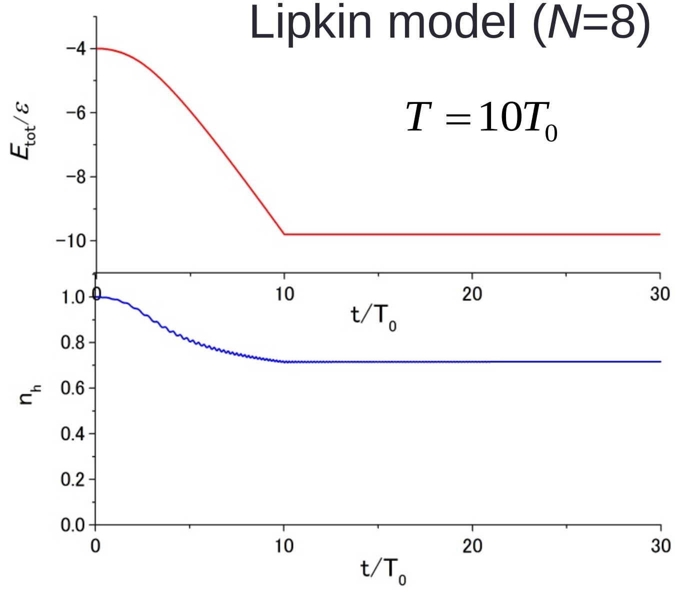
$$\Rightarrow\begin{cases}(\varepsilon_{\alpha}-\varepsilon_{\alpha'})n_{\alpha\alpha'}+\sum_{\lambda_1\lambda_2\lambda_3}\left\{\langle\alpha\lambda_3|v|\lambda_1\lambda_2\rangle C_{\lambda_1\lambda_2\alpha'\lambda_3}-C_{\alpha\lambda_3\lambda_1\lambda_2}\langle\lambda_1\lambda_2|v|\alpha'\lambda_3\rangle\right\}=0\\(\varepsilon_{\alpha}+\varepsilon_{\beta}-\varepsilon_{\alpha'}-\varepsilon_{\beta'})C_{\alpha\beta\alpha'\beta'}+B_{\alpha\beta\alpha'\beta'}+P_{\alpha\beta\alpha'\beta'}+H_{\alpha\beta\alpha'\beta'}+T_{\alpha\beta\alpha'\beta'}=0\end{cases}$$

Adiabatic method is convenient:

Starting from HF ground state, we solve TDDM equations with slowly increasing interaction

$$\boxed{v \Rightarrow v \times \frac{t}{T} \quad \text{with } T >> T_0 = \frac{2\pi\hbar}{\varepsilon}}$$

Lipkin model (N=8)



Excited-state calculation

- Small amplitude limit of TDDM (STDDM)
- Equation-of-motion approach

Small amplitude limit of TDDM (STDDM)

$$|\Psi(t)\rangle \approx |\Psi_0\rangle + \lambda \sum e^{-i\omega_\mu t/\hbar} |\Psi_\mu\rangle, \qquad \lambda << 1$$

$$i\hbar \frac{d}{dt} n_{\alpha\alpha'} = i\hbar \frac{d}{dt} \langle \Psi(t) | a^+_{\alpha'} a_\alpha | \Psi(t) \rangle = \langle \Psi(t) | [a^+_{\alpha'} a_\alpha, H] | \Psi(t) \rangle$$

$$\approx \lambda \sum \left(\omega_\mu \langle \Psi_0 | a^+_{\alpha'} a_\alpha | \Psi_\mu \rangle e^{-i\omega_\mu t/\hbar} - \omega_\mu \langle \Psi_\mu | a^+_{\alpha'} a_\alpha | \Psi_0 \rangle e^{i\omega_\mu t/\hbar} \right)$$

$$= \lambda \sum \left(\langle \Psi_0 | [a^+_{\alpha'} a_\alpha, H] | \Psi_\mu \rangle e^{-i\omega_\mu t/\hbar} + \langle \Psi_\mu | [a^+_{\alpha'} a_\alpha, H] | \Psi_0 \rangle e^{i\omega_\mu t/\hbar} \right)$$

$$\Downarrow$$

$$\langle \Psi_0 | [a^+_{\alpha'} a_\alpha, H] | \Psi_\mu \rangle = \omega_\mu \underline{\langle \Psi_0 | a^+_{\alpha'} a_\alpha | \Psi_\mu \rangle} = \omega_\mu \tilde{x}^\mu_{\alpha\alpha'}$$

$\tilde{x}^\mu_{\alpha\alpha'}$: Transition amplitude

$$\left\langle \Psi_0 \left| [a^+_{\alpha'} a_\alpha , H] \right| \Psi_\mu \right\rangle = (\varepsilon_\alpha - \varepsilon_{\alpha'}) \tilde{x}^\mu_{\alpha\alpha'} + \sum_{\lambda\lambda_1\lambda_1'} \Big(\langle \alpha\lambda_1 | v | \lambda\lambda_1' \rangle_A n_{\lambda\alpha'} - \langle \lambda\lambda_1 | v | \alpha'\lambda_1' \rangle_A n_{\alpha\lambda} \Big) \tilde{x}^\mu_{\lambda_1'\lambda_1}$$

$$+ \sum_{\lambda_2\lambda_1'\lambda_2'} \langle \alpha\lambda_2 | v | \lambda_1'\lambda_2' \rangle \tilde{X}^\mu_{\lambda_1'\lambda_2'\alpha'\lambda_2} - \sum_{\lambda_1\lambda_2\lambda_2'} \langle \lambda_1\lambda_2 | v | \alpha'\lambda_2' \rangle \tilde{X}^\mu_{\alpha\lambda_2'\lambda_1\lambda_2}$$

$$= \omega_\mu \tilde{x}^\mu_{\alpha\alpha'}$$

$$\begin{pmatrix} n_h = 1 \\ n_p = 0 \\ \tilde{X}^\mu_{\alpha\beta\alpha'\beta'} = 0 \end{pmatrix} \longrightarrow \quad \tilde{x}^\mu_{\alpha\alpha'} = \begin{pmatrix} x^\mu_{mi} \\ -y^\mu_{mi} \end{pmatrix}$$

RPA

Similarly for C_2

$$i\hbar\frac{d}{dt}C_{\alpha\beta\alpha'\beta'} = i\hbar\frac{d}{dt}\left\langle\Psi(t)\middle| a^{+}_{\alpha'}a^{+}_{\beta'}a_{\beta}a_{\alpha}\middle|\Psi(t)\right\rangle = \left\langle\Psi(t)\middle|[a^{+}_{\alpha'}a^{+}_{\beta'}a_{\beta}a_{\alpha}, H]\middle|\Psi(t)\right\rangle$$

$$\Rightarrow \left\langle\Psi_0\middle|[a^{+}_{\alpha'}a^{+}_{\beta'}a_{\beta}a_{\alpha}, H]\middle|\Psi_\mu\right\rangle = \omega_\mu\left\langle\Psi_0\middle| a^{+}_{\alpha'}a^{+}_{\beta'}a_{\beta}a_{\alpha}\middle|\Psi_\mu\right\rangle = \omega_\mu\tilde{X}^{\mu}_{\alpha\beta\alpha'\beta'}$$

STDDM equation

$$\begin{pmatrix} a & c \\ b & d \end{pmatrix}\begin{pmatrix} \tilde{x}^{\mu} \\ \tilde{X}^{\mu} \end{pmatrix} = \omega_\mu\begin{pmatrix} \tilde{x}^{\mu} \\ \tilde{X}^{\mu} \end{pmatrix}$$

Equation-of-motion approach

$$Q_\mu^+ = \sum_{\lambda\lambda'} x_{\lambda\lambda'}^\mu a_\lambda^+ a_{\lambda'} + \sum_{\lambda_1\lambda_2\lambda_1'\lambda_2'} X_{\lambda\lambda'}^\mu a_{\lambda_1}^+ a_{\lambda_2}^+ a_{\lambda_2'} a_{\lambda_1'} : \qquad Q_\mu^+ \left|\Psi_0\right\rangle = \left|\Psi_\mu\right\rangle, \qquad Q_\mu \left|\Psi_0\right\rangle = 0$$

$$\left\langle \Psi_0 \right| [a_{\alpha'}^+ a_\alpha, H] \left| \Psi_\mu \right\rangle = (E_\mu - E_0) \left\langle \Psi_0 \right| a_{\alpha'}^+ a_\alpha \left| \Psi_\mu \right\rangle = \omega_\mu \left\langle \Psi_0 \right| a_{\alpha'}^+ a_\alpha \left| \Psi_\mu \right\rangle$$

$$\left\langle \Psi_0 \right| [a_{\alpha'}^+ a_{\beta'}^+ a_\beta a_\alpha, H] \left| \Psi_\mu \right\rangle = \omega_\mu \left\langle \Psi_0 \right| a_{\alpha'}^+ a_{\beta'}^+ a_\beta a_\alpha \left| \Psi_\mu \right\rangle$$

$$\Downarrow$$

$$\boxed{\begin{pmatrix} A & B \\ C & D \end{pmatrix} \begin{pmatrix} x^\mu \\ X^\mu \end{pmatrix} = \omega_\mu \begin{pmatrix} S_1 & T_1 \\ T_2 & S_2 \end{pmatrix} \begin{pmatrix} x^\mu \\ X^\mu \end{pmatrix}}$$

$$A = \left\langle \Psi_0 \right| [[a_{\alpha'}^+ a_\alpha, H], a_\lambda^+ a_{\lambda'}] \left| \Psi_0 \right\rangle \qquad S_1 = \left\langle \Psi_0 \right| [a_{\alpha'}^+ a_\alpha, a_\lambda^+ a_{\lambda'}] \left| \Psi_0 \right\rangle$$

$$B = \left\langle \Psi_0 \right| [[a_{\alpha'}^+ a_\alpha, H], a_{\lambda_1}^+ a_{\lambda_2}^+ a_{\lambda_2'} a_{\lambda_1'}] \left| \Psi_0 \right\rangle \qquad T_1 = \left\langle \Psi_0 \right| [a_{\alpha'}^+ a_\alpha, a_{\lambda_1}^+ a_{\lambda_2}^+ a_{\lambda_2'} a_{\lambda_1'}] \left| \Psi_0 \right\rangle$$

$$C = \left\langle \Psi_0 \right| [[a_{\alpha'}^+ a_{\beta'}^+ a_\beta a_\alpha, H], a_\lambda^+ a_{\lambda'}] \left| \Psi_0 \right\rangle \qquad T_2 = \left\langle \Psi_0 \right| [a_{\alpha'}^+ a_{\beta'}^+ a_\beta a_\alpha, a_\lambda^+ a_{\lambda'}] \left| \Psi_0 \right\rangle$$

$$D = \left\langle \Psi_0 \right| [[a_{\alpha'}^+ a_{\beta'}^+ a_\beta a_\alpha, H], a_{\lambda_1}^+ a_{\lambda_2}^+ a_{\lambda_2'} a_{\lambda_1'}] \left| \Psi_0 \right\rangle \qquad S_2 = \left\langle \Psi_0 \right| [a_{\alpha'}^+ a_{\beta'}^+ a_\beta a_\alpha, a_{\lambda_1}^+ a_{\lambda_2}^+ a_{\lambda_2'} a_{\lambda_1'}] \left| \Psi_0 \right\rangle$$

Extended second RPA (ESRPA)

Under HF assumption

$$\begin{pmatrix} n_h = 1 \\ n_p = 0 \\ C_2 = 0 \end{pmatrix} \longrightarrow$$

Second RPA (SRPA)

SRPA operator

$$Q_\mu^+ = \sum_{mi} x_{mi}^\mu a_m^+ a_i - \sum_{mi} y_{mi}^\mu a_i^+ a_m + \sum_{mnij} X_{mnij}^\mu a_m^+ a_n^+ a_j a_i - \sum_{mnij} Y_{mnij}^\mu a_i^+ a_j^+ a_n a_m$$

i, *j*   : hole states
m, *n* : particle states

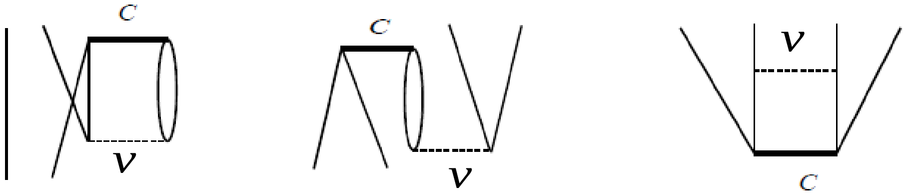
One-body part of ESRPA (1b-ESRPA)

$$\boxed{Ax^{\mu} = \omega_{\mu} S_1 x^{\mu}}$$

$$S_1 = (n_{\alpha'} - n_{\alpha})\delta_{\alpha\lambda}\delta_{\alpha'\lambda'}$$

$$A = [(\varepsilon_{\alpha} - \varepsilon_{\alpha'})\delta_{\alpha\lambda}\delta_{\alpha'\lambda'} + (n_{\lambda'} - n_{\lambda})\langle \alpha\lambda' | v | \alpha'\lambda \rangle](n_{\alpha'} - n_{\alpha})$$

$$+ \delta_{\alpha\lambda} \sum_{\gamma\gamma'\gamma''} \langle \gamma\gamma' | v | \alpha'\gamma'' \rangle C_{\lambda'\gamma''\gamma\gamma'} + \sum_{\gamma\gamma'} \langle \lambda'\gamma | v | \alpha'\gamma' \rangle_A C_{\alpha\gamma'\lambda\gamma} - \sum_{\gamma\gamma'} \langle \gamma\gamma' | v | \alpha'\lambda \rangle C_{\alpha\lambda'\gamma\gamma'} + \cdots$$

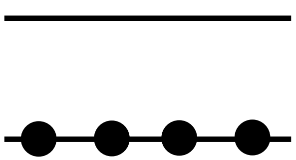


Self-energy

Vertex corrections

3）Applications

Lipkin model



$$H = \varepsilon\, J_0 + \frac{V}{2}\left(J_+^2 + J_-^2\right)$$

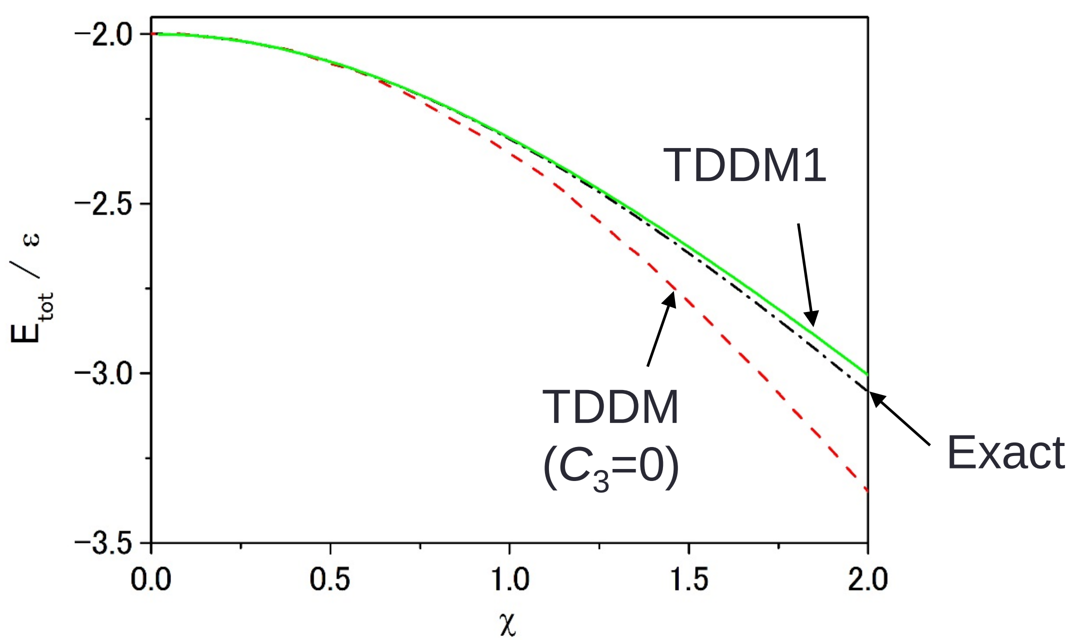
$$J_0 = \frac{1}{2}\sum_{p=1}^{N}(a_p^+ a_p - a_{-p}^+ a_{-p}), \quad J_+ = J_-^+ = \sum_{p=1}^{N} a_p^+ a_{-p}$$

For $\chi = \dfrac{(N-1)|V|}{\varepsilon} \leq 1 \qquad \left|\mathrm{HF}\right\rangle = \prod_{p=1}^{N} a_{-p}^+ \left|0\right\rangle$

For $\chi > 1 \qquad \left|\mathrm{DHF}(\alpha)\right\rangle = \prod_{p=1}^{N} c_{-p}^+ \left|0\right\rangle$

$$\begin{pmatrix} c_{-p} \\ c_p \end{pmatrix} = \begin{pmatrix} \cos\alpha & \sin\alpha \\ -\sin\alpha & \cos\alpha \end{pmatrix} \begin{pmatrix} a_{-p} \\ a_p \end{pmatrix} \quad , \ \cos 2\alpha = 1/\chi$$

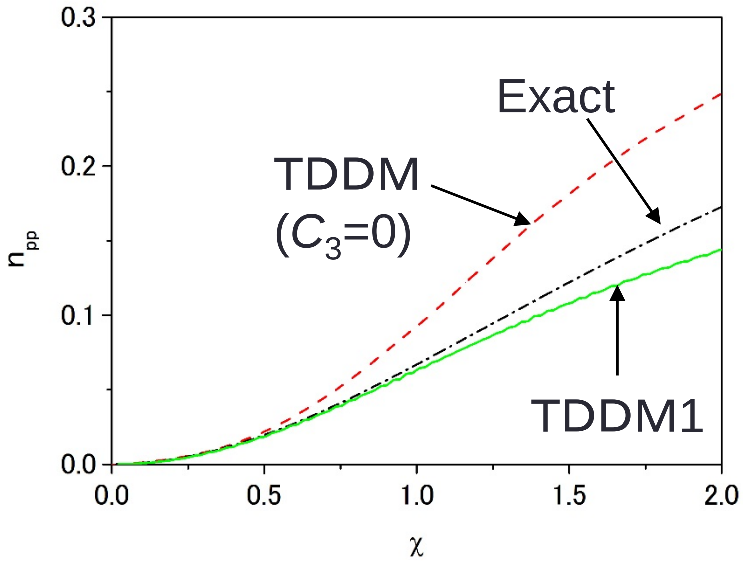
Ground state energy N=4



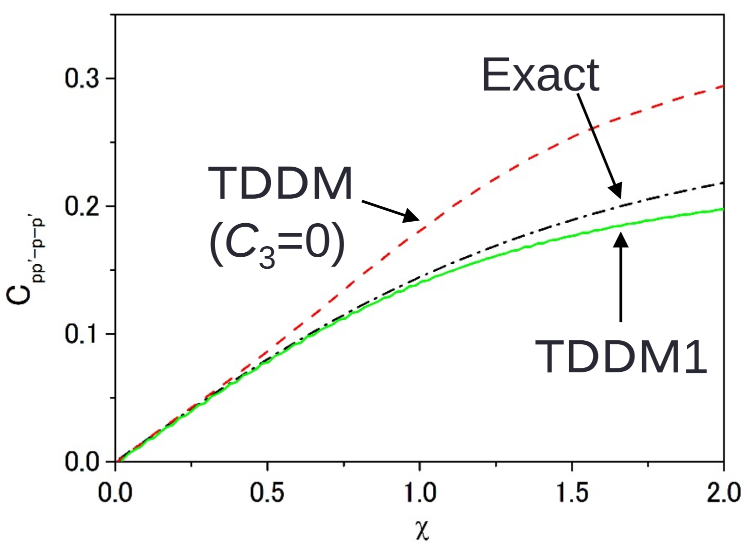
$$\chi = (N-1)\frac{|V|}{\varepsilon}$$

N=4

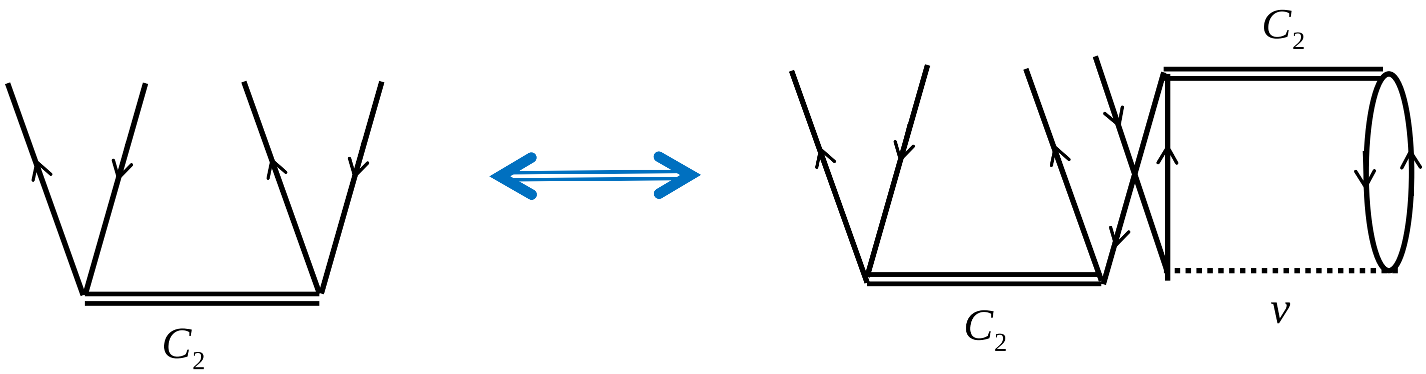
Occupation probability



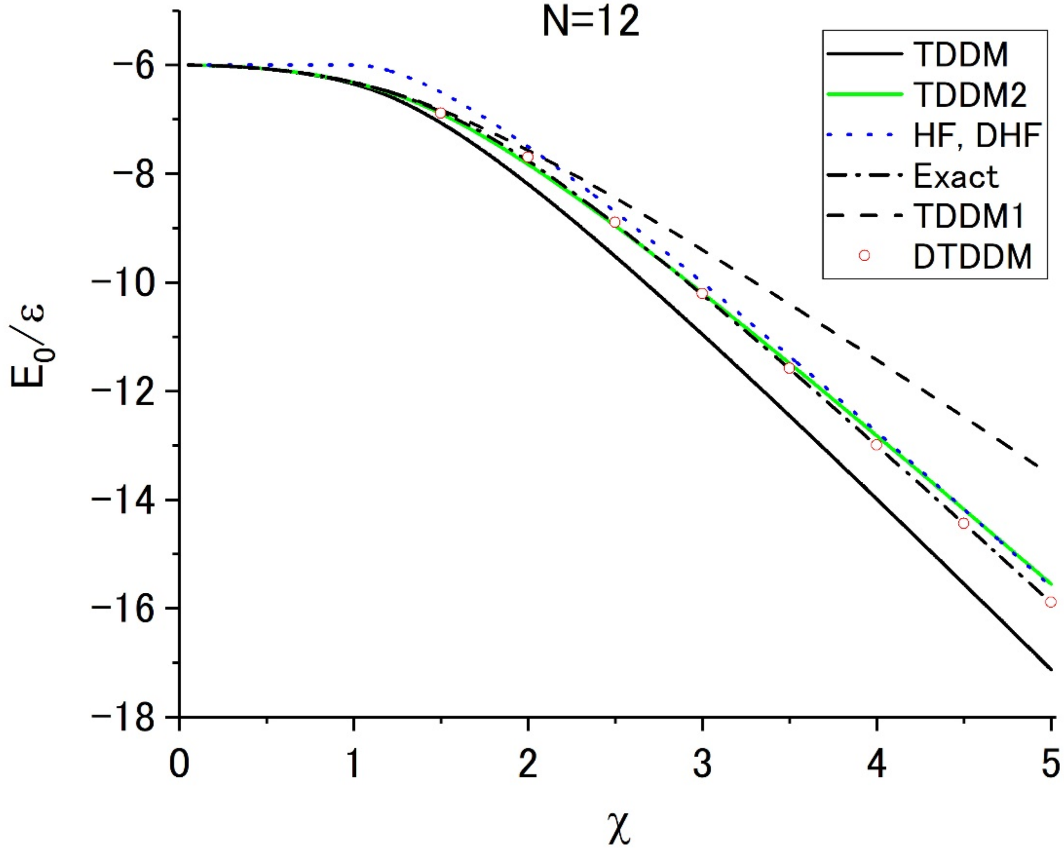
Correlation matrix C_2



Self-energy contributions from C_3 suppress excess correlations



$$C_3 \approx C_2 \times C_2$$

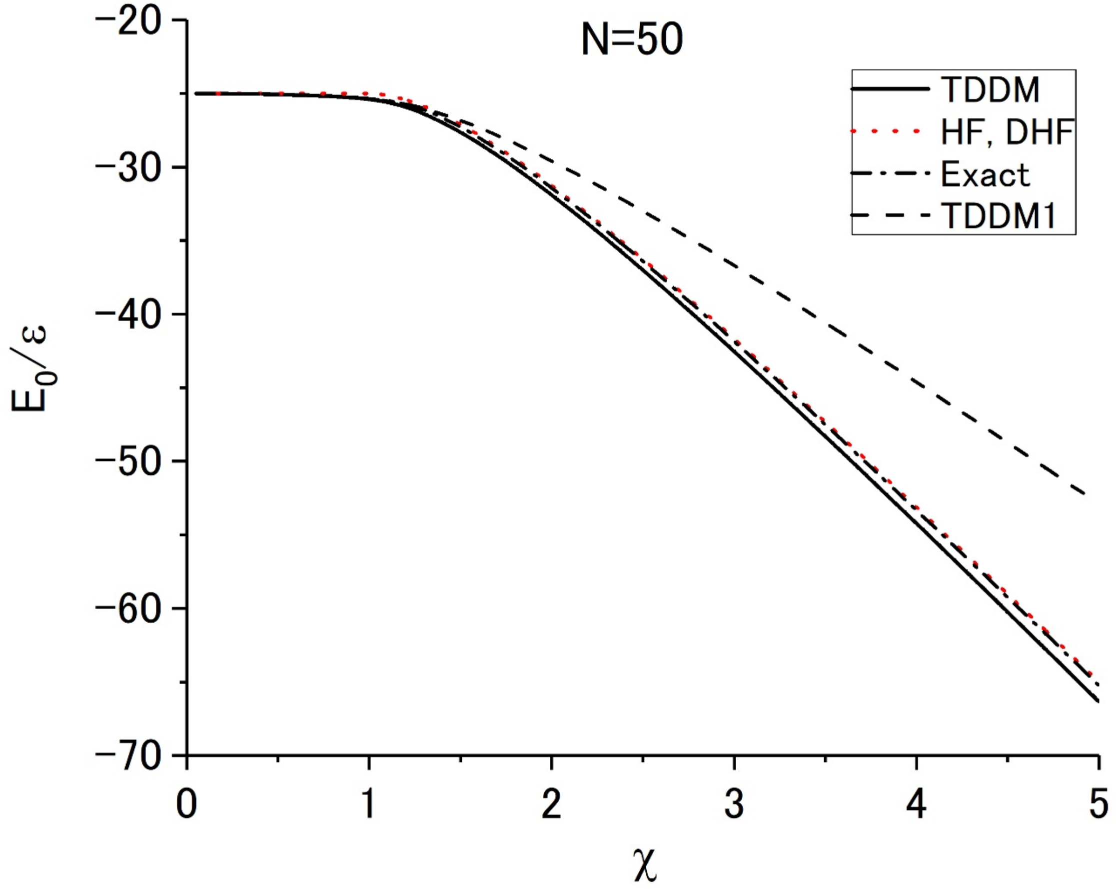


TDDM2:

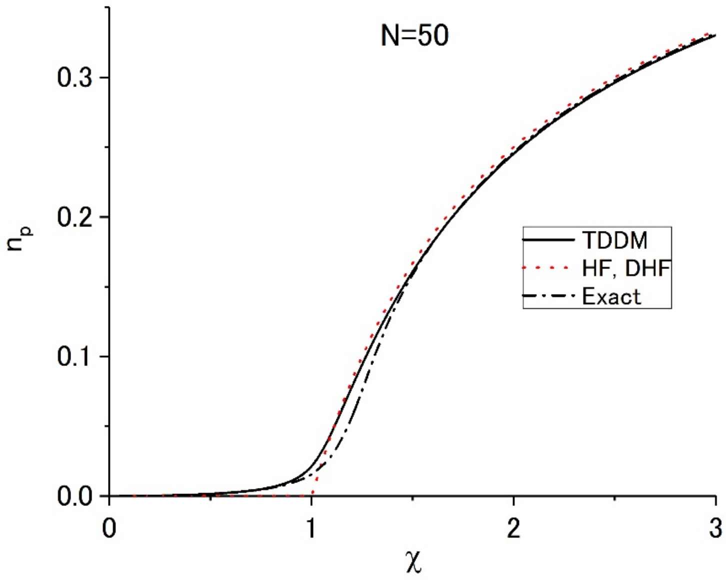
$$C_{p_1p_2h_1p_3p_4h_2} \approx \frac{1}{N}\sum_h C_{hh_1p_3p_4}C_{p_1p_2h_2h}$$

$$C_{p_1h_1h_2p_2h_3h_4} \approx \frac{1}{N}\sum_p C_{h_1h_2p_2p}C_{p_1ph_3h_4}$$

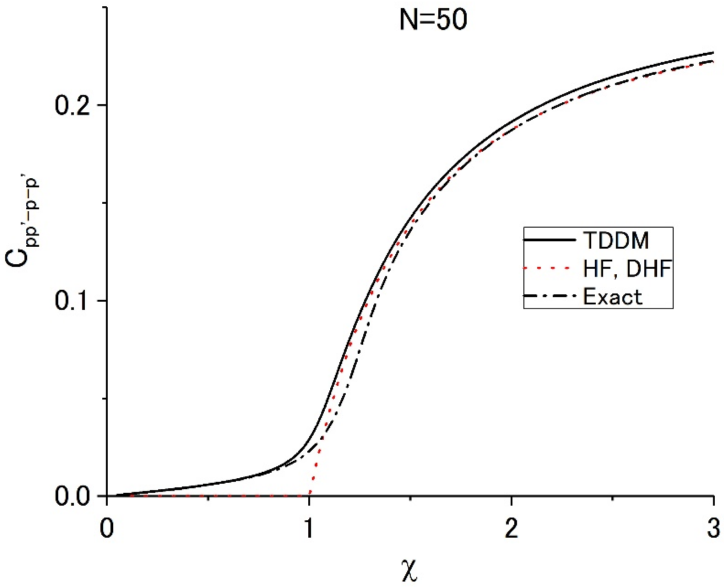
$$N = 1 + \frac{1}{4}\sum_{pp'hh'} C_{pp'hh'}C^*_{pp'hh'}$$


N=50
TDDM
HF, DHF
Exact
TDDM1
−20
−30
−40
−50
−60
−70
0
1
2
3
4
5
E_0/ε
χ

Occupation probability



Correlation matrix C_2



$$C_{pp'-p-p'}(\mathrm{DHF}) = (n_{p-p}(\mathrm{DHF}))^2$$

Deformed HF (DHF) is good approximation for large *N* and χ

$$|\Phi_0\rangle \approx \frac{1}{\sqrt{2}}(|\mathrm{DHF}(\alpha)\rangle + |\mathrm{DHF}(-\alpha)\rangle), \quad \cos 2\alpha = \frac{1}{\chi}$$

$$n_p = \langle\Phi_0|a_p^+ a_p|\Phi_0\rangle \approx \frac{1}{2}(\langle\mathrm{DHF}(\alpha)|a_p^+ a_p|\mathrm{DHF}(\alpha)\rangle + \langle\mathrm{DHF}(-\alpha)|a_p^+ a_p|\mathrm{DHF}(-\alpha)\rangle) = n_p(\mathrm{DHF})$$

$$n_{p-p} = \langle\Phi_0|a_{-p}^+ a_p|\Phi_0\rangle \approx \frac{1}{2}(\langle\mathrm{DHF}(\alpha)|a_{-p}^+ a_p|\mathrm{DHF}(\alpha)\rangle + \langle\mathrm{DHF}(-\alpha)|a_{-p}^+ a_p|\mathrm{DHF}(-\alpha)\rangle) = 0$$

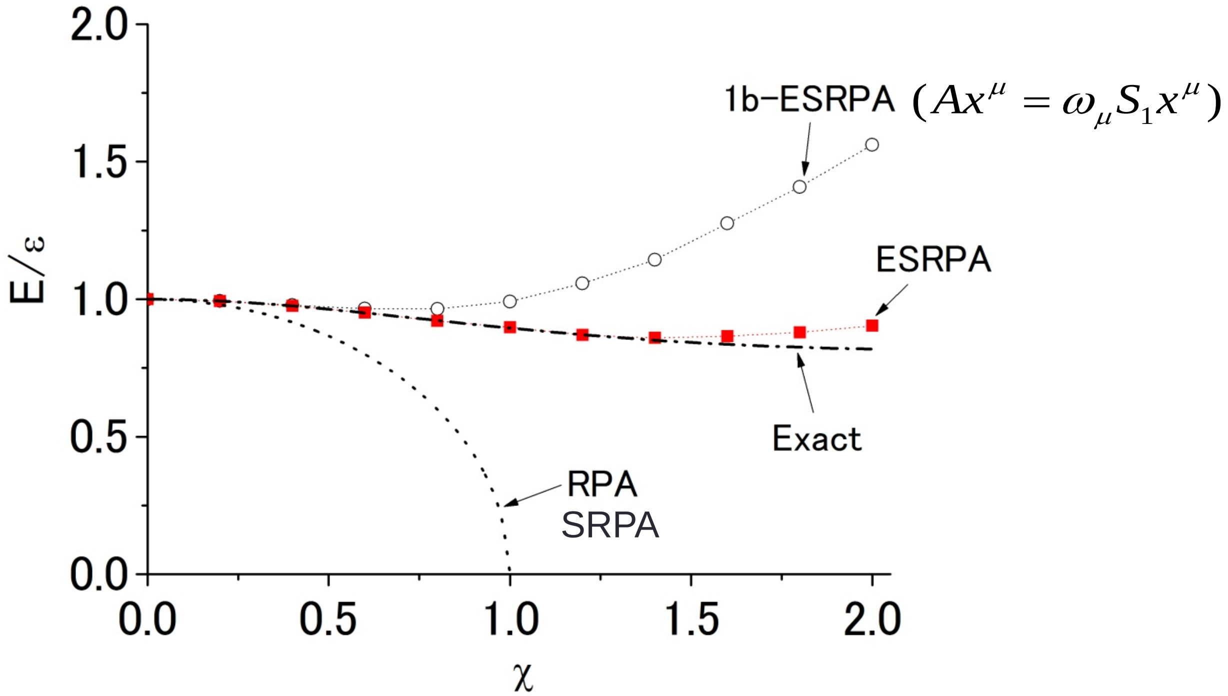
$$\rho_{pp'-p-p'} = \langle\Phi_0|a_{-p}^+ a_{-p'}^+ a_{p'} a_p|\Phi_0\rangle = C_{pp'-p-p'} \approx (n_{p-p}(\mathrm{DHF}))^2$$

$$\rho_{pp'p''p-p'-p''} = \langle\Phi_0|a_p^+ a_{-p'}^+ a_{-p''}^+ a_{p''} a_{p'} a_p|\Phi_0\rangle \approx n_p(\mathrm{DHF})(n_{p-p}(\mathrm{DHF}))^2 = n_p C_{pp'-p-p'}$$

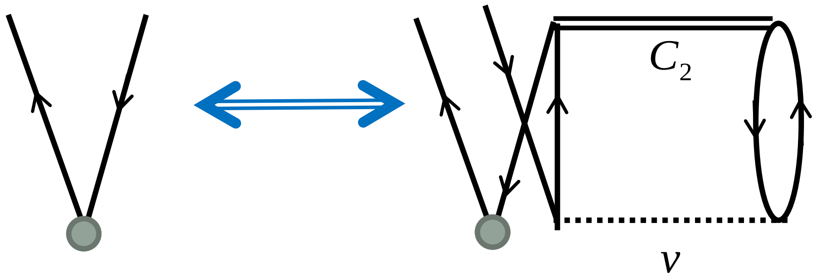
$$\downarrow$$

TDDM with $C_3 = 0$ becomes good

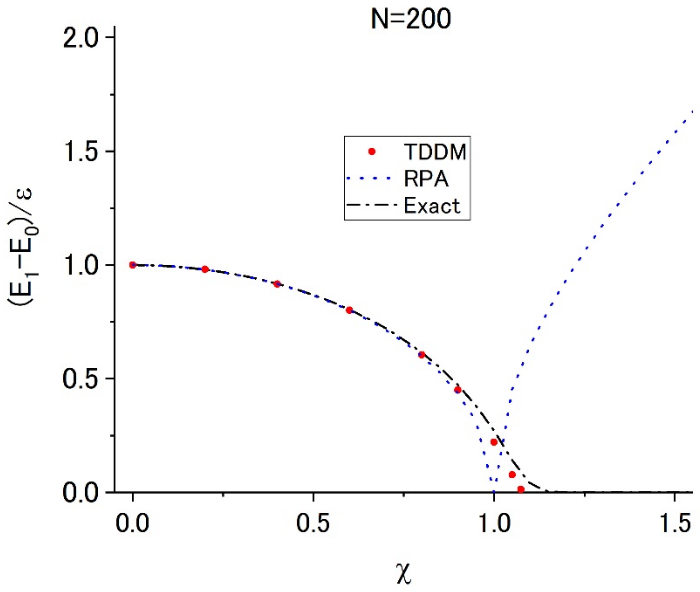
Excited states N=4

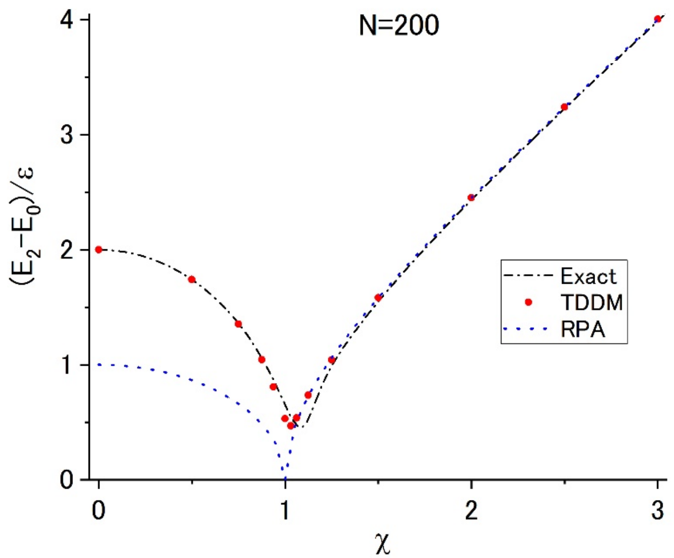


Self-energy contributions
in 1b-ESRPA



Excited states in STDDM (N=200, C_3=0)



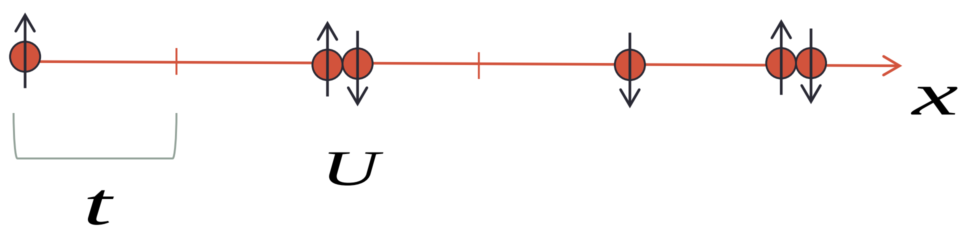


1D-Hubbard model (*N*=6 at half-filling)

$$H = -t\sum_{\langle i,j\rangle,\sigma} c^{+}_{i,\sigma}c_{j,\sigma} + U\sum_{i}\hat{n}_{i\uparrow}\hat{n}_{i\downarrow} \quad , \qquad \hat{n}_{i\sigma} = c^{+}_{i,\sigma}c_{i,\sigma}$$

hopping

on-site repulsion

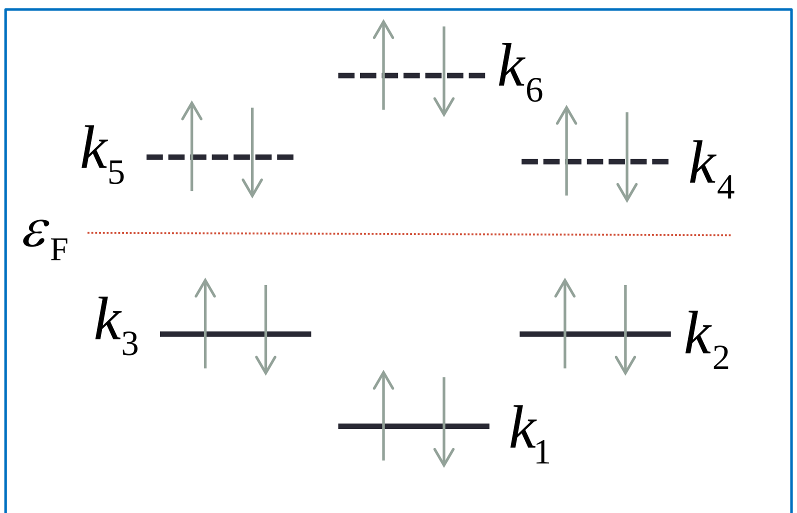


In momentum space

$$c_{i,\sigma} = \frac{1}{\sqrt{N}} \sum_k a_{k,\sigma} e^{ikx_i}$$

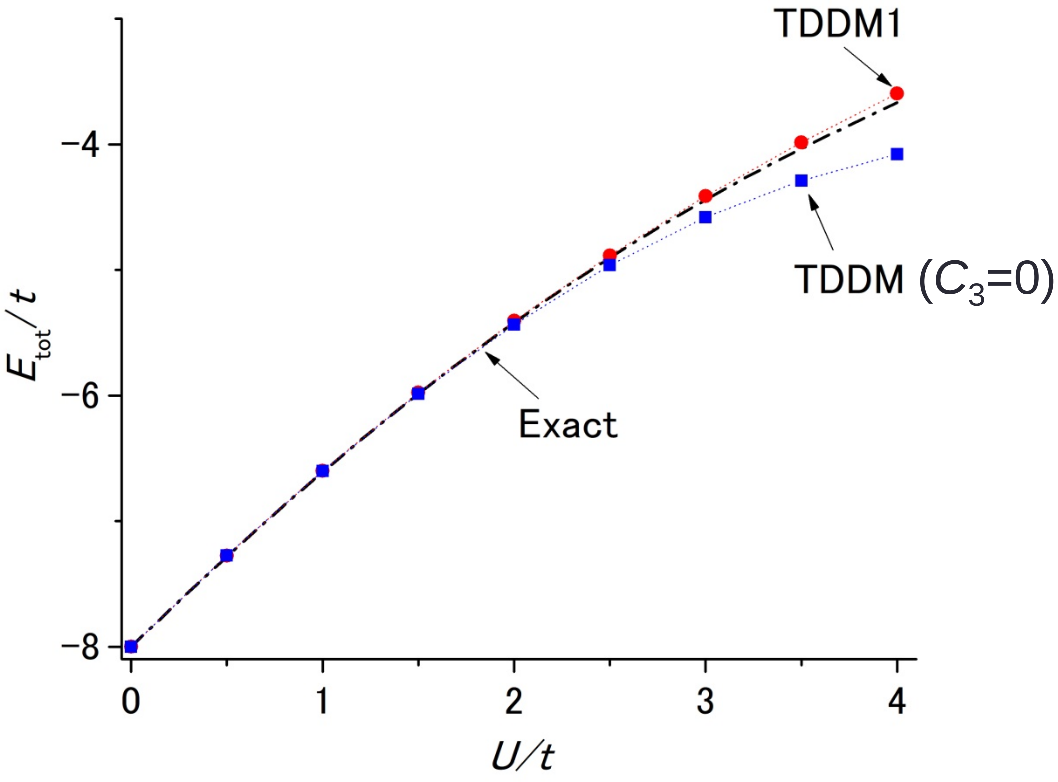
$$H = \sum_{k,\sigma} \varepsilon_k a^{+}_{k,\sigma} a_{k,\sigma} + \frac{U}{2N} \sum_{k,p,q,\sigma} a^{+}_{k,\sigma} a_{k+q,\sigma} a^{+}_{p,-\sigma} a_{p-q,-\sigma}$$

$$\varepsilon_k = -2t\cos k_k \ , \ k_1 = 0, \ k_{2,3} = \pm\frac{\pi}{3}, \ k_{4,5} = \pm\frac{2\pi}{3}, \ k_6 = -\pi$$



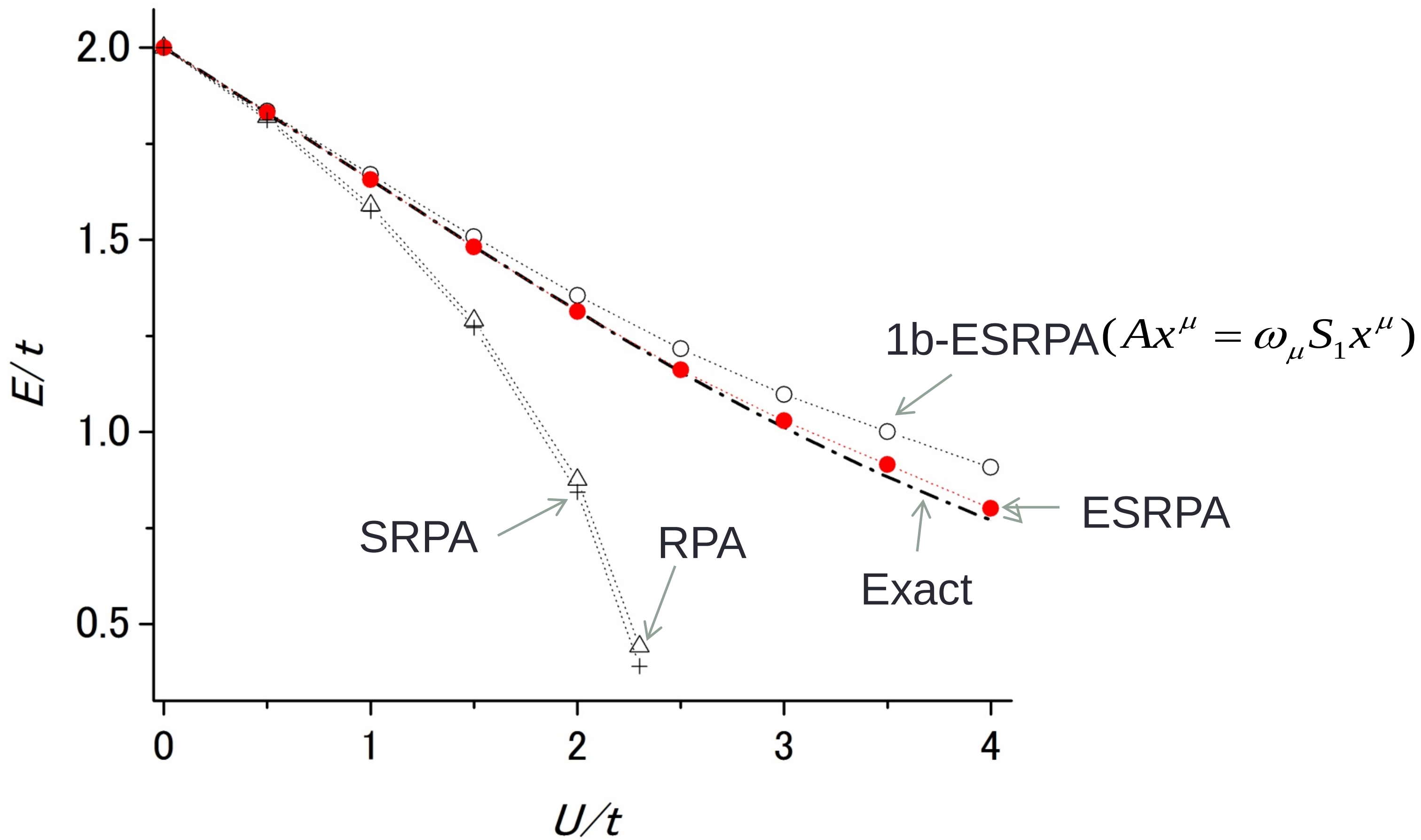
$$\left|\mathrm{HF}\right\rangle = \prod_{i=1,\sigma}^{3} a^{+}_{k_i,\sigma} \left|0\right\rangle$$

Ground state energy (N=6)



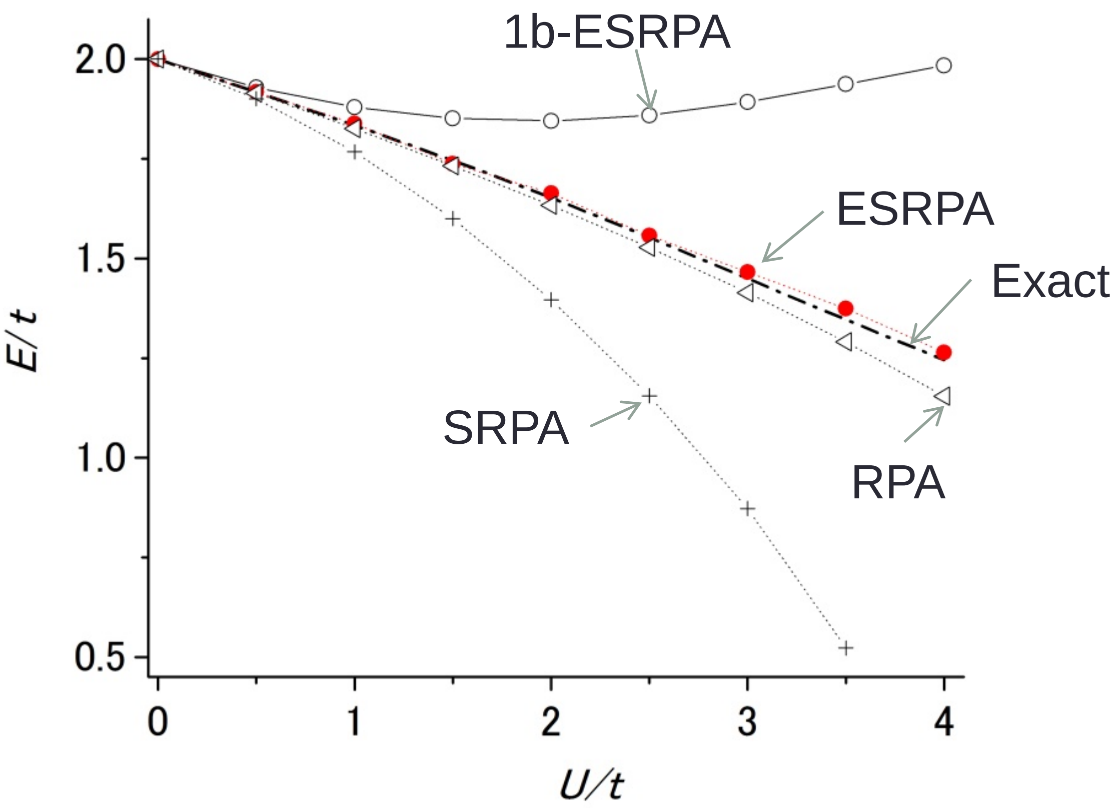
1st excited state (spin mode)

$$\Delta q = \pi : \left(-\frac{\pi}{3} \uparrow \Rightarrow \frac{2\pi}{3} \uparrow \right) - \left(-\frac{\pi}{3} \downarrow \Rightarrow \frac{2\pi}{3} \downarrow \right)$$



2nd excited state (spin mode)

$$\Delta q = \frac{\pi}{3} : \left(\frac{\pi}{3} \uparrow \Rightarrow \frac{2\pi}{3} \uparrow \right) - \left(\frac{\pi}{3} \downarrow \Rightarrow \frac{2\pi}{3} \downarrow \right)$$



Self-energy + coupling to X^{μ} are important

E1 and E2 excitations in ^{40}Ca and ^{48}Ca

Ground-state calculations (TDDM)

Single-particle states:

$$1d_{5/2}\,,1d_{3/2}\,,2s_{1/2}\,,1f_{7/2}\,(\underbrace{1f_{5/2}\,,2p_{3/2}\,,2p_{1/2}}_{^{48}\mathrm{Ca}})\ \text{ for } n_{\alpha\alpha}\ \text{ and } C_{pp'hh'}$$

Residual interaction: simplified Skyrme III

$$v_2 = t_0(1+x_0P_\sigma)\delta^3(\vec{r}-\vec{r}\,')\,,\ v_3 = t_3\delta^3(\vec{r}-\vec{r}\,')\,\delta^3(\vec{r}-\vec{r}\,'')$$

Occupation probabilities

^{40}Ca

	ϵ_α [MeV]		$n_{\alpha\alpha}$	
orbit	proton	neutron	proton	neutron
$1d_{5/2}$	-15.6	-22.9	0.923	0.924
$1d_{3/2}$	-9.4	-16.5	0.884	0.884
$2s_{1/2}$	-8.5	-15.9	0.846	0.846
$1f_{7/2}$	-3.4	-10.4	0.154	0.154

^{48}Ca

	ϵ_α [MeV]		$n_{\alpha\alpha}$	
orbit	proton	neutron	proton	neutron
$1d_{5/2}$	-22.6	-22.4	0.963	0.965
$1d_{3/2}$	-17.1	-17.0	0.952	0.940
$2s_{1/2}$	-15.1	-16.4	0.905	0.932
$1f_{7/2}$	-10.6	-10.6	0.059	0.919
$2p_{3/2}$	-1.7	-3.8	-	0.103
$2p_{1/2}$	0.1	-2.0	-	0.064
$1f_{5/2}$	-2.2	-1.9	0.022	0.116

Excited-state calculations (STDDM)

Single-particle states:

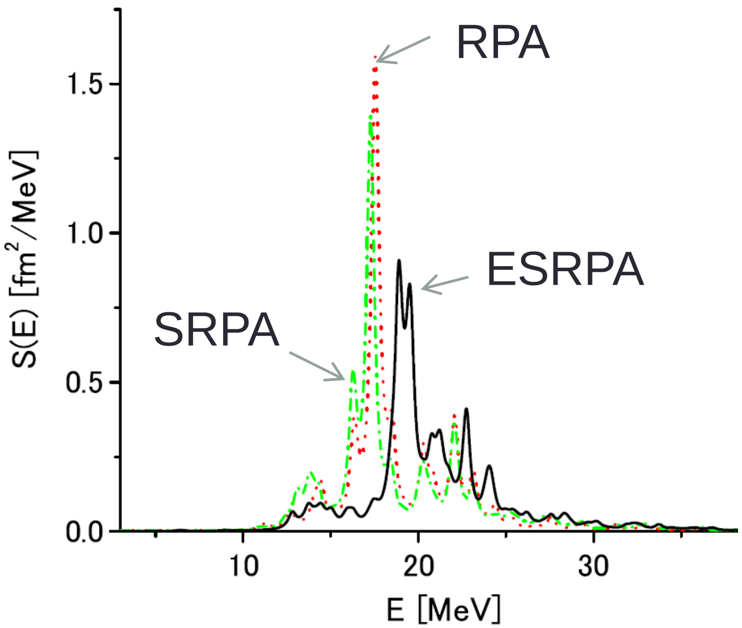
for $x^{\mu}_{\alpha\alpha'} : \varepsilon_{\alpha} \leq 50\ \mathrm{MeV}\ ,\ \ell \leq 11/2$

for $X^{\mu}_{pp'hh'} : 2p_{3/2}\ ,\ 2p_{1/2}\ ,\ 1d_{5/2}\ ,\ 1d_{3/2}\ ,\ 2s_{1/2}\ ,\ 1f_{7/2}\ (\underbrace{1f_{5/2}\ ,\ 2p_{3/2}\ ,\ 2p_{1/2}}_{^{48}\mathrm{Ca}})$

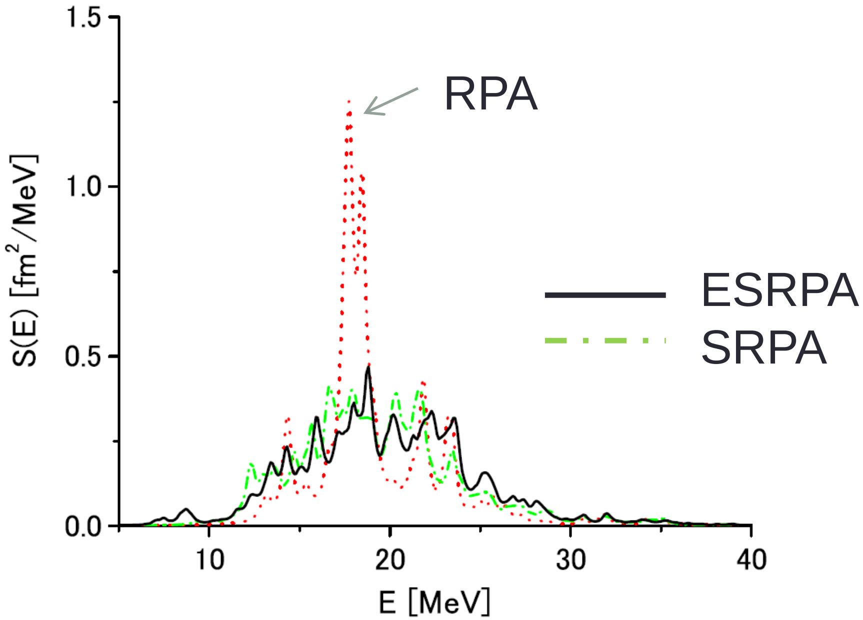
Residual interaction: simplified Skyrme III

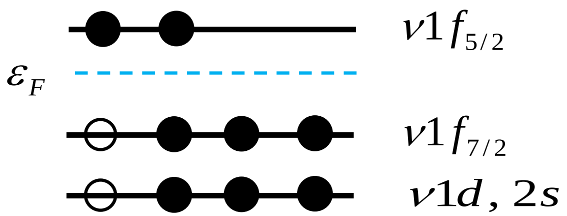
$$v_2 = t_0(1 + x_0 P_\sigma)\delta^3(\vec{r} - \vec{r}')\ ,\ v_3 = t_3 \delta^3(\vec{r} - \vec{r}')\ \delta^3(\vec{r} - \vec{r}'')$$

^{40}Ca *E*1

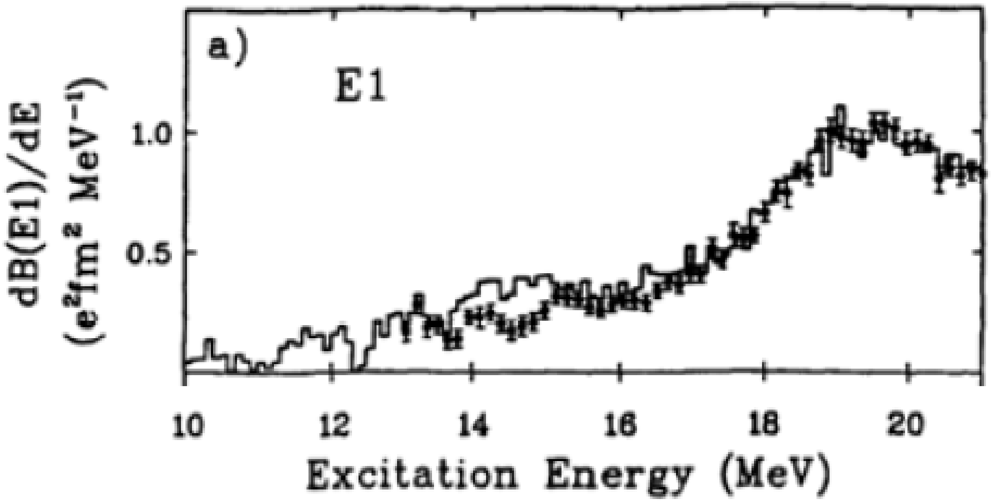


^{48}Ca *E*1





$^{40}Ca(e,e'x)$

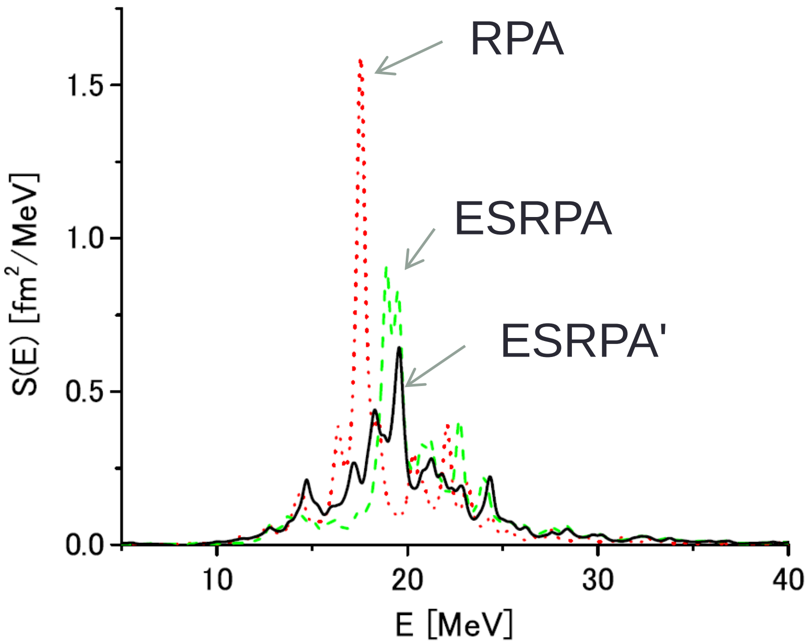


H. Diesner et al. Phys. Rev.Lett. 72, 1994(1994)

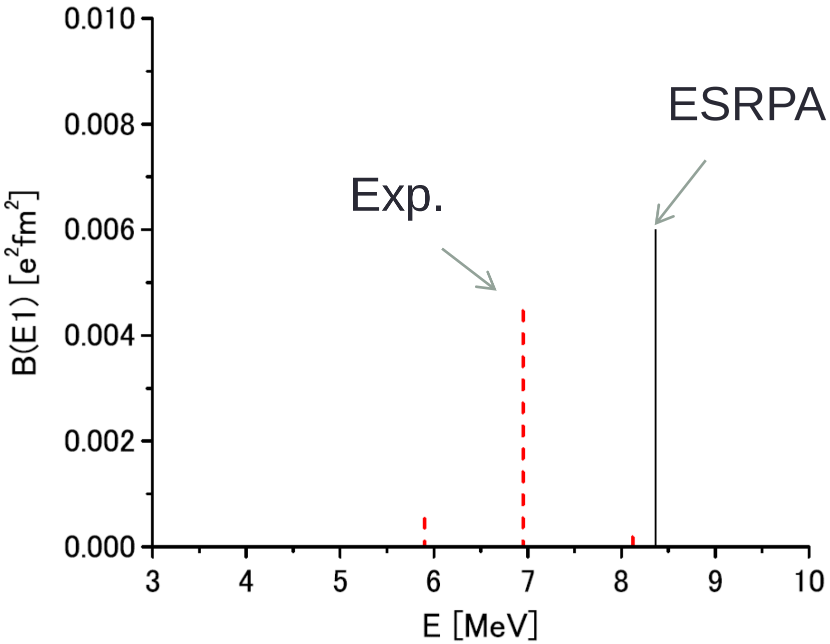
Contributions of 3p-1h and 1p-3h states in ^{40}Ca

Norm matrix for 3p-1h state: $S_2 \approx (1-n_p)(1-n_{p'})n_{p''}n_h \neq 0$

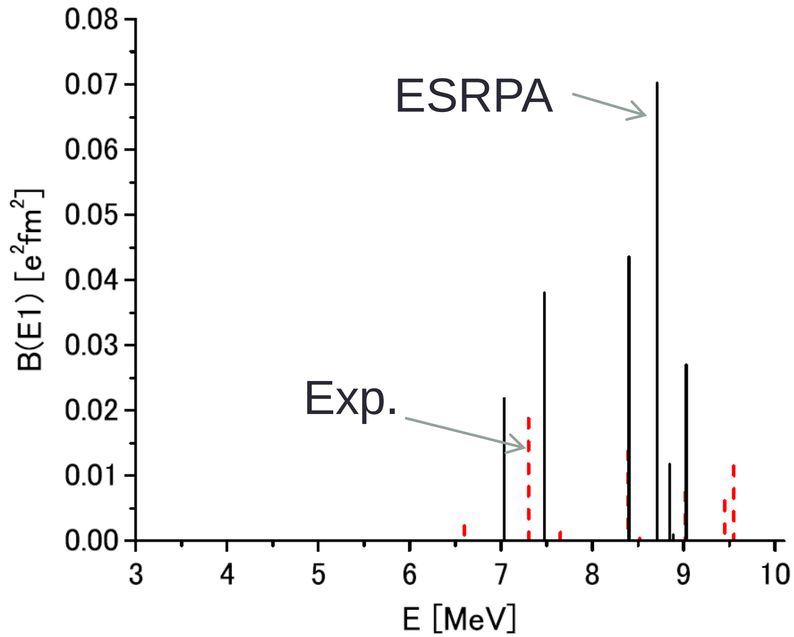
ESRPA' : $X^{\mu}_{pp'hh'} + X^{\mu}_{hh'pp'} + X^{\mu}_{pp'p''h} + X^{\mu}_{phh'h''} + \cdots$



^{40}Ca E1

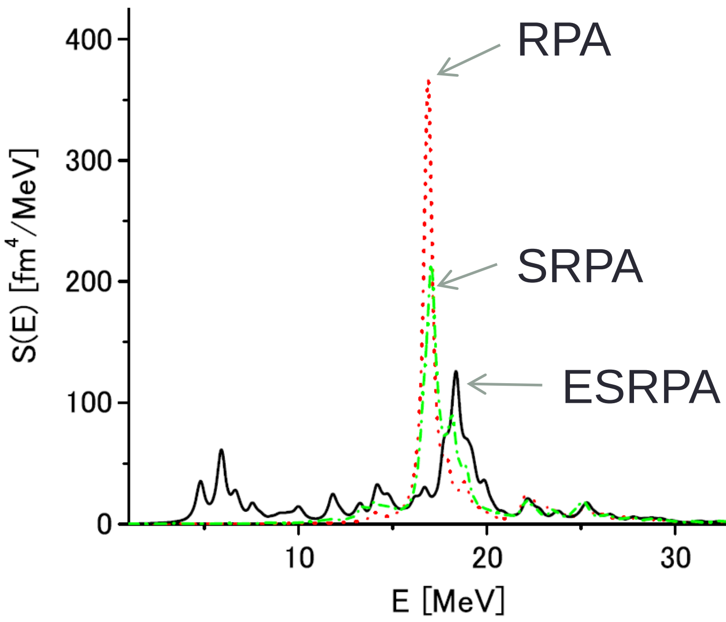


^{48}Ca E1

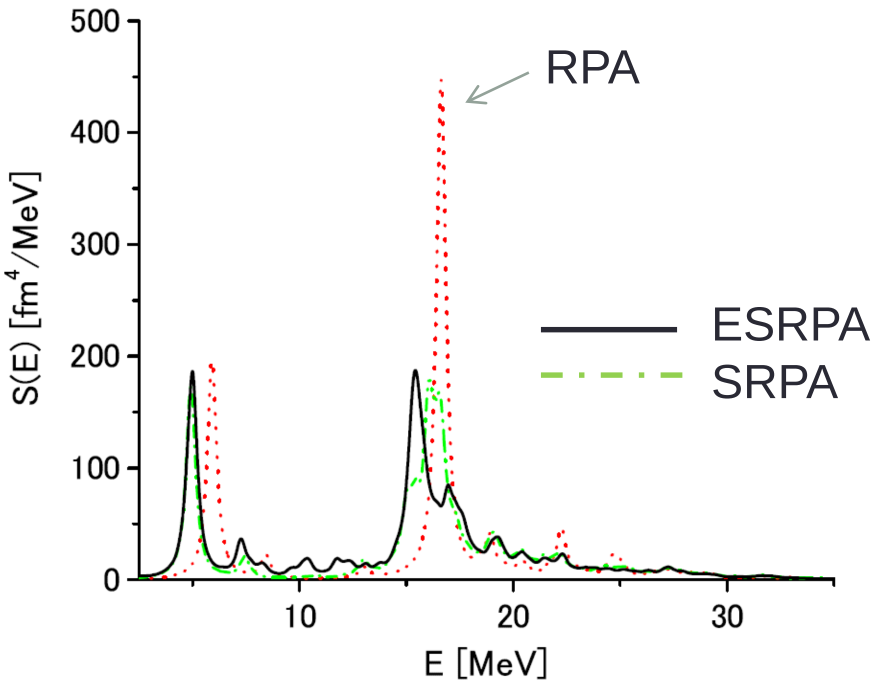


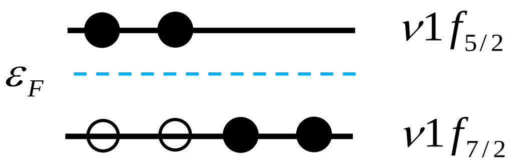
T. Hartmann et al., Phys. Rev. Lett. 85, 274(2000)

^{40}Ca *E*2

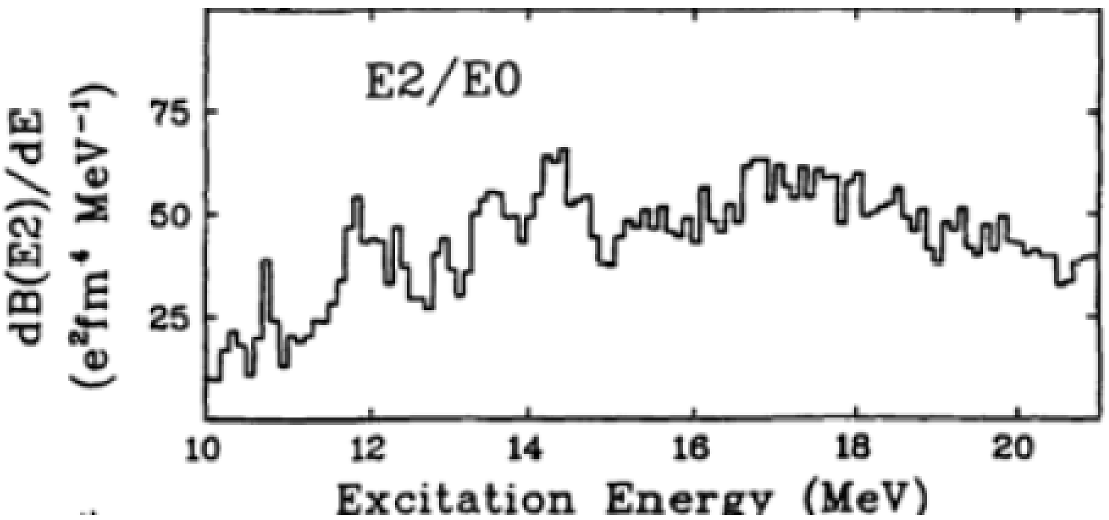


^{48}Ca *E*2





$^{40}Ca(e,e'x)$

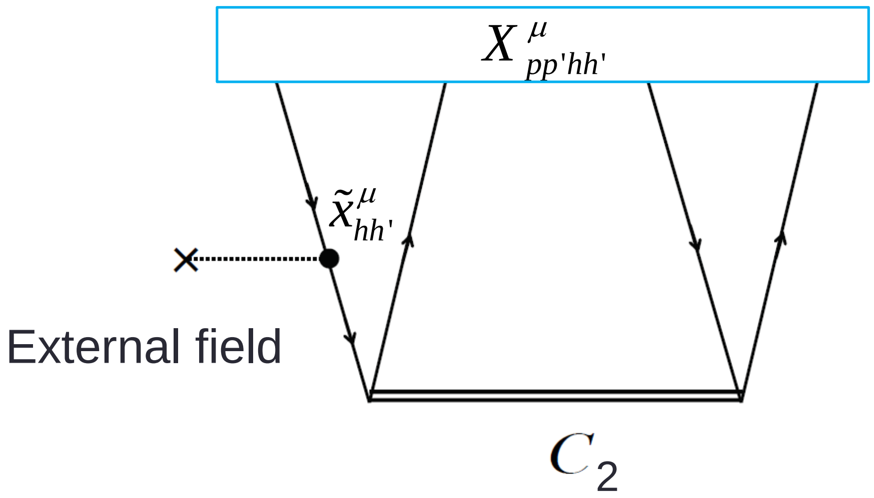


H. Diesner et al. Phys. Rev. Lett. 72, 1994(1994)

Reasons for strong fragmentation in ^{40}Ca

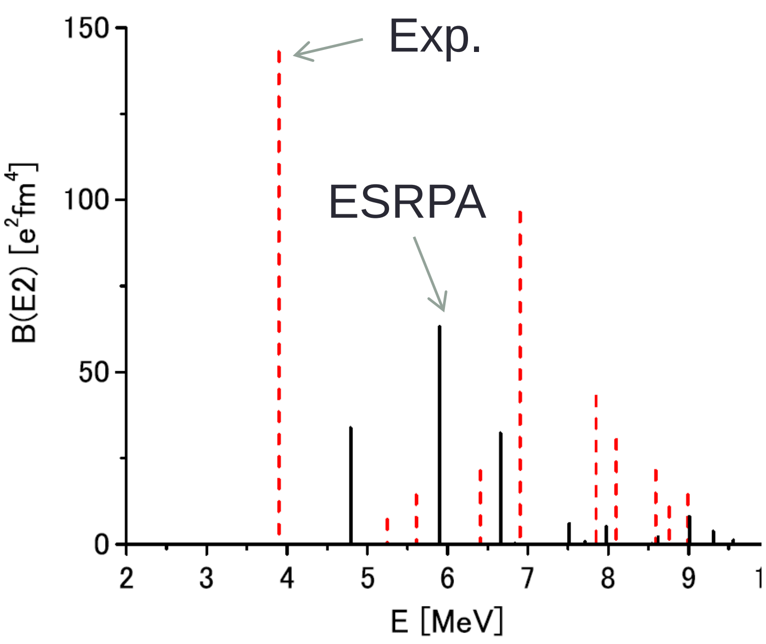
- Partial occupation of $1f_{7/2}$ states

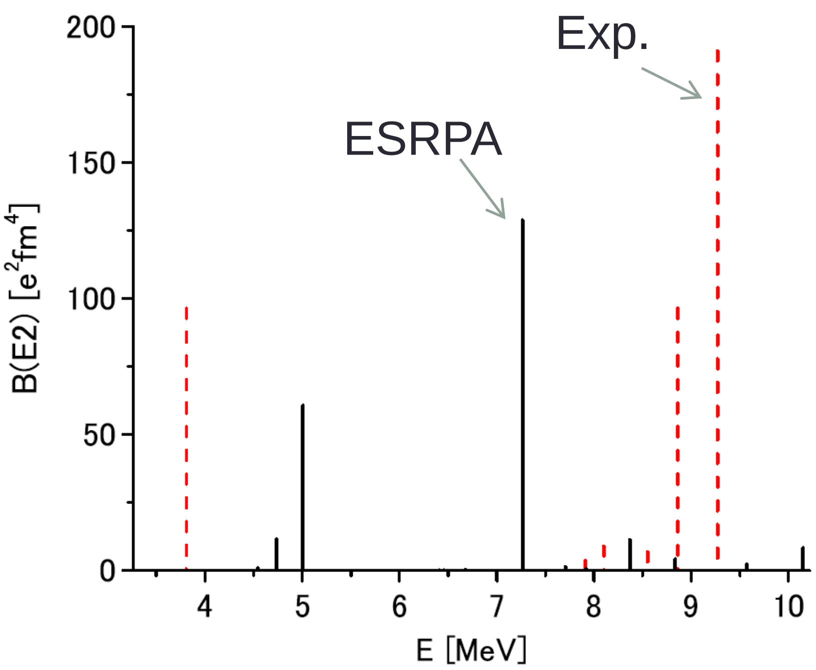
- Contributions of h-h and p-p amplitudes



^{40}Ca *E*2

^{48}Ca *E*2





T. Hartmann et al., Phys. Rev. Lett. 85, 274(2000)

4) Summary

- TDDM is a straightforward extension of TDHF

- $C_3 \approx C_2 \times C_2$ gives a better truncation scheme of BBGKY hierarchy except for large *N* Lipkin model.

- TDDM g.s. +ESRPA works for solvable models

  Excited states :self-energy + coupling to $X^{\mu}_{\alpha\beta\alpha'\beta'}$ are important

- Ground-state correlations are important for fragmentation of *E*1 and *E*2 strengths in ^{40}Ca and ^{48}Ca

Ortho-normalization condition in ESRPA

$$\begin{pmatrix} x^{\mu *} & X^{\mu *} \end{pmatrix} \begin{pmatrix} S_1 & T_1 \\ T_2 & S_2 \end{pmatrix} \begin{pmatrix} x^{\nu} \\ X^{\nu} \end{pmatrix} = \delta_{\mu\nu}$$

$\begin{pmatrix} x^{\mu *} & X^{\mu *} \end{pmatrix}$: left eigen vector

Relation of ESRPA and STDDM

$$\begin{pmatrix} \tilde{x}^{\mu} \\ \tilde{X}^{\mu} \end{pmatrix} \approx \begin{pmatrix} S_1 & T_1 \\ T_2 & S_2 \end{pmatrix} \begin{pmatrix} x^{\mu} \\ X^{\mu} \end{pmatrix}$$

STDDM ESRPA