Progress in density-matrix theory and applications

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１）Time-dependent density-matrix theory (TDDM)
- Ground state
- Excited states

２）Applications
- Lipkin model
- 1D Hubbard model
- E1 and E2 excitations of ^{40}Ca and ^{48}Ca

3） Summary

1）Time-dependent density-matrix theory (TDDM)

Hamiltonian:

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

1-body and 2-body density matrices:

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

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

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

Equations of motion:

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

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

BBGKY hierarchy

$$i\hbar\dot{n}_{\alpha\alpha'} = (\varepsilon_\alpha - \varepsilon_{\alpha'})n_{\alpha\alpha'} + \sum_{\lambda\lambda'\lambda''}\left[\langle\alpha\lambda|v|\lambda'\lambda''\rangle C_{\lambda'\lambda''\alpha'\lambda} - C_{\alpha\lambda\lambda'\lambda''}\langle\lambda'\lambda''|v|\alpha'\lambda\rangle\right]$$

$$i\hbar\dot{C}_{\alpha\beta\alpha'\beta'} = (\varepsilon_\alpha + \varepsilon_\beta - \varepsilon_{\alpha'} - \varepsilon_{\beta'})C_{\alpha\beta\alpha'\beta'} + B_{\alpha\beta\alpha'\beta'} + P_{\alpha\beta\alpha'\beta'} + H_{\alpha\beta\alpha'\beta'} + T_{\alpha\beta\alpha'\beta'}$$

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

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

2p-2h excitation

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

pp(hh) correlation

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

ph correlation

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

coupling to C_3

- Simple truncation scheme (TDDM'):

$$C_3 = 0$$

(Wang & Cassing, Ann. Phys. 159, 328('85))

- New truncation scheme:

$$C_{p_1p_2h_1p_3p_4h_2} \approx \sum_h C_{hh_1p_3p_4} C_{p_1p_2h_2h}$$

$$C_{p_1h_1h_2p_2h_3h_4} \approx \sum_p C_{h_1h_2p_2p} C_{p_1ph_3h_4}$$

(Tohyama & Schuck, Eur. Phys. J. A 50, 7('14))

CCD-like ground state

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

gives

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

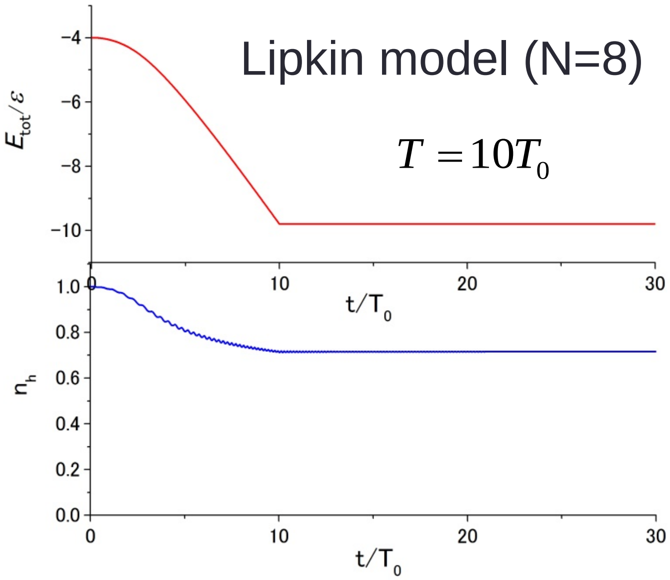
$$C_{p_1p_2h_1p_3p_4h_2} \approx \sum_h z^*_{p_3p_4hh_1} z_{p_1p_2h_2h}, \; C_{p_1h_1h_2p_2h_3h_4} \approx \sum_p z^*_{p_2ph_1h_2} z_{p_1ph_3h_4}$$

Ground state: a stationary solution of TDDM eqs.

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

Adiabatic method starting from HF ground state

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



Excited states : Equation of motion approach

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

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

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

↓

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

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

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

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

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

Extended second RPA (ESRPA)

Under HF assumption

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

Second RPA (SRPA)

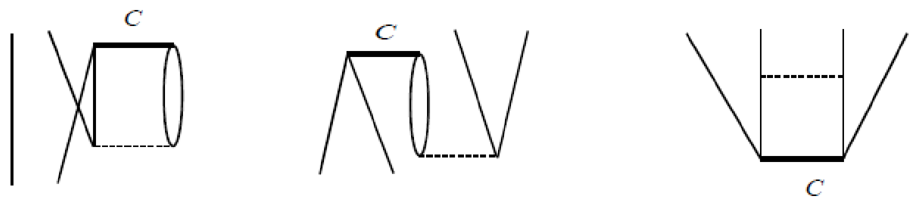
$$\left(x^{\mu}_{ph},\ x^{\mu}_{hp},\ X^{\mu}_{pp'hh'},\ X^{\mu}_{hh'pp'} \right)$$

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

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

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

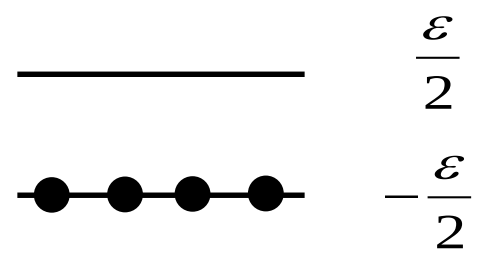
$$A = [(\varepsilon_{\alpha} - \varepsilon_{\alpha'})\delta_{\alpha\lambda}\delta_{\alpha'\lambda'} + (n_{\lambda'} - n_{\lambda})\langle \alpha\lambda' | v | \alpha'\lambda \rangle](n_{\alpha'} - n_{\alpha})$$
$$+ \delta_{\alpha\lambda} \sum_{\gamma\gamma'\gamma''} \langle \gamma\gamma' | v | \alpha'\gamma''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



Self-energy Vertex corrections

2）Applications

Lipkin model

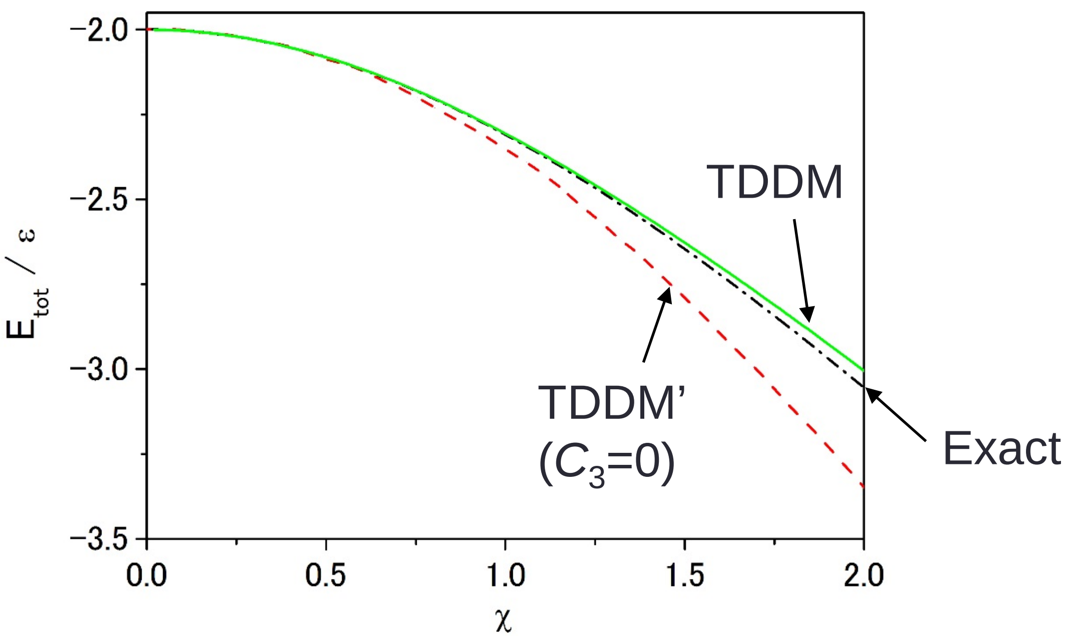


$$H = \varepsilon J_0 + \frac{V}{2}\left(J_+^2 + J_-^2\right)$$

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

$$J_+ = J_-^+ = \sum_{p=1}^{N} a_p^+ a_{-p}$$

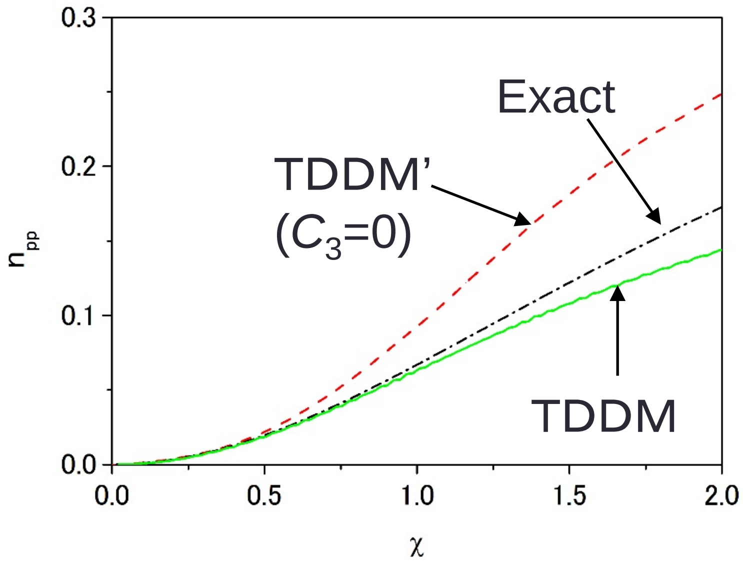
Ground state energy *N*=4



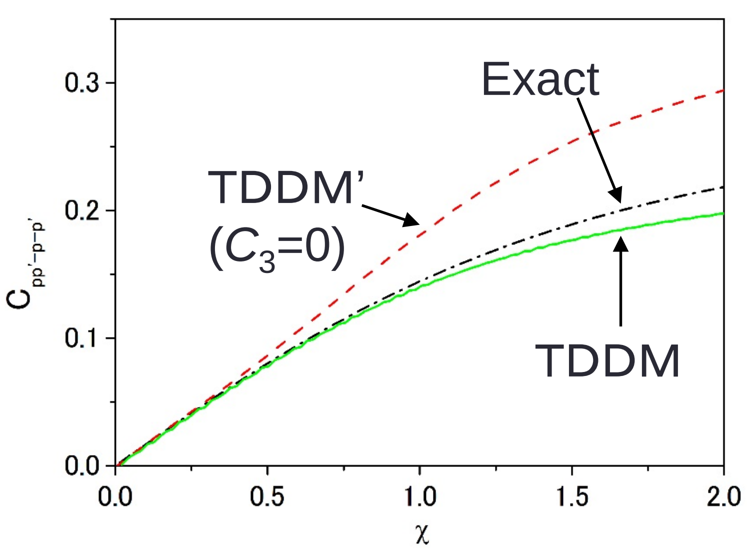
$$\chi = (N-1)\frac{|V|}{\varepsilon}$$

N=4

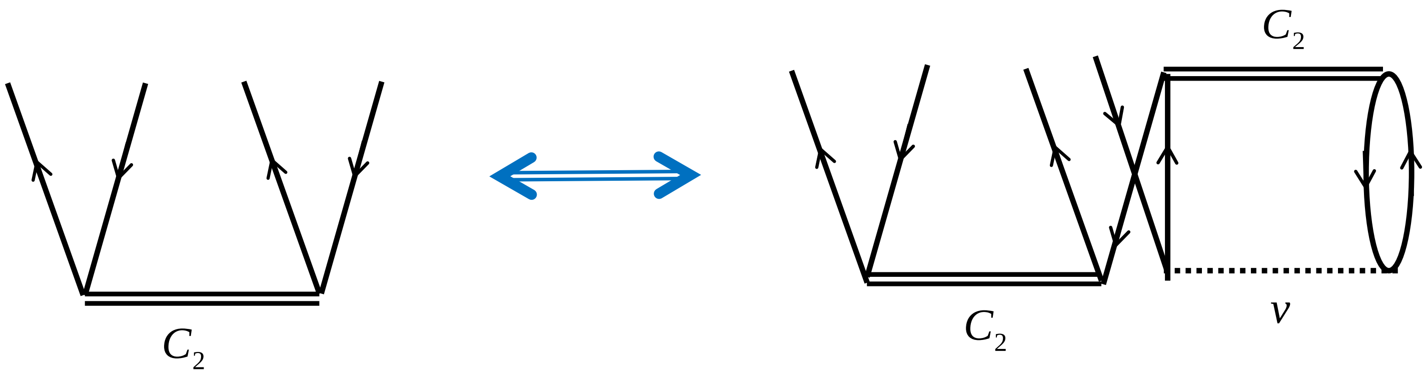
Occupation probability



Correlation matrix C_2

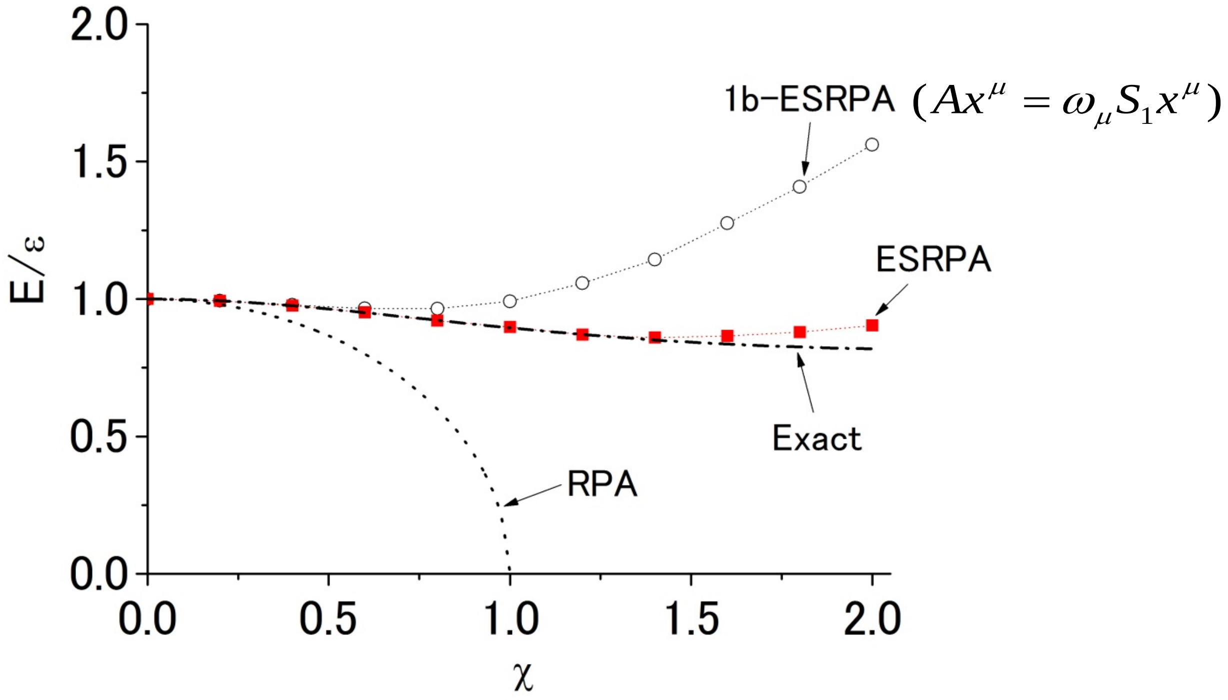


Self-energy contributions from C_3 suppress excess correlations

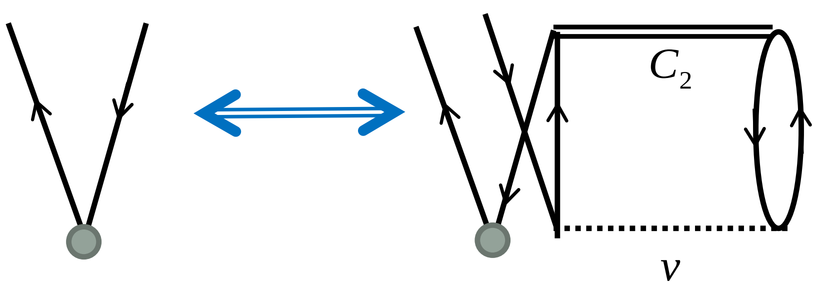


$$C_3 \approx C_2 \times C_2$$

Excited states *N*=4



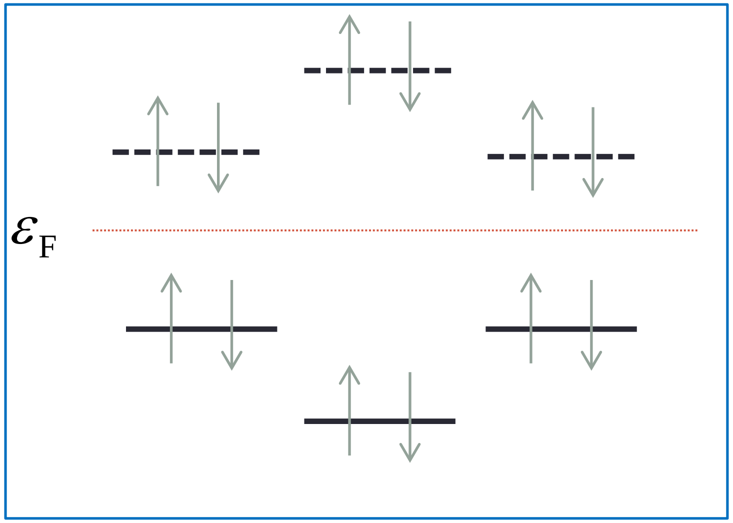
Self-energy contributions
in 1b-ESRPA



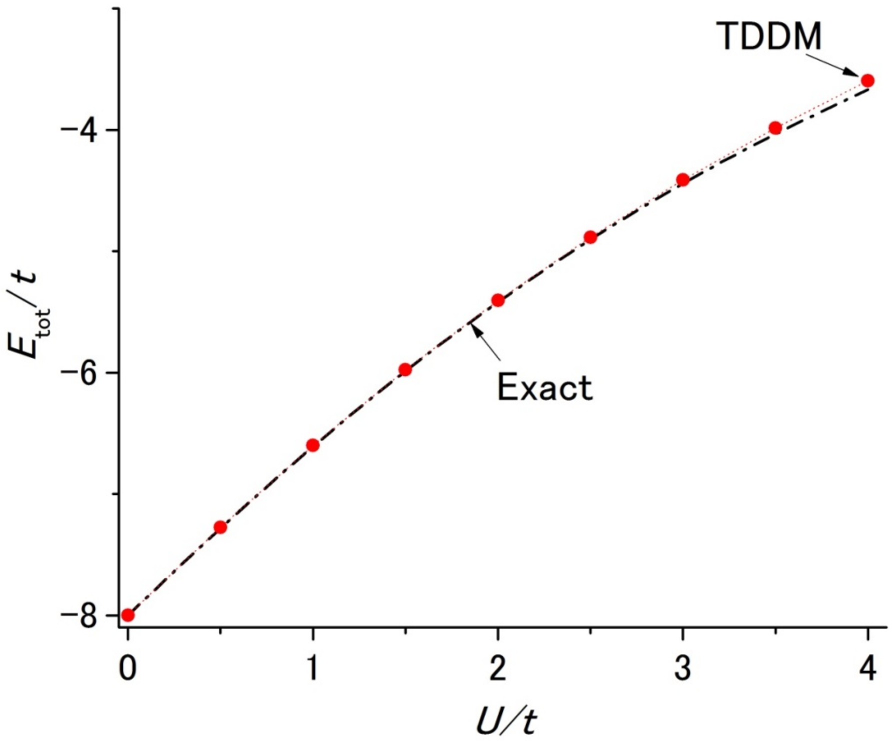
1D-Hubbard model (N=6)

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

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

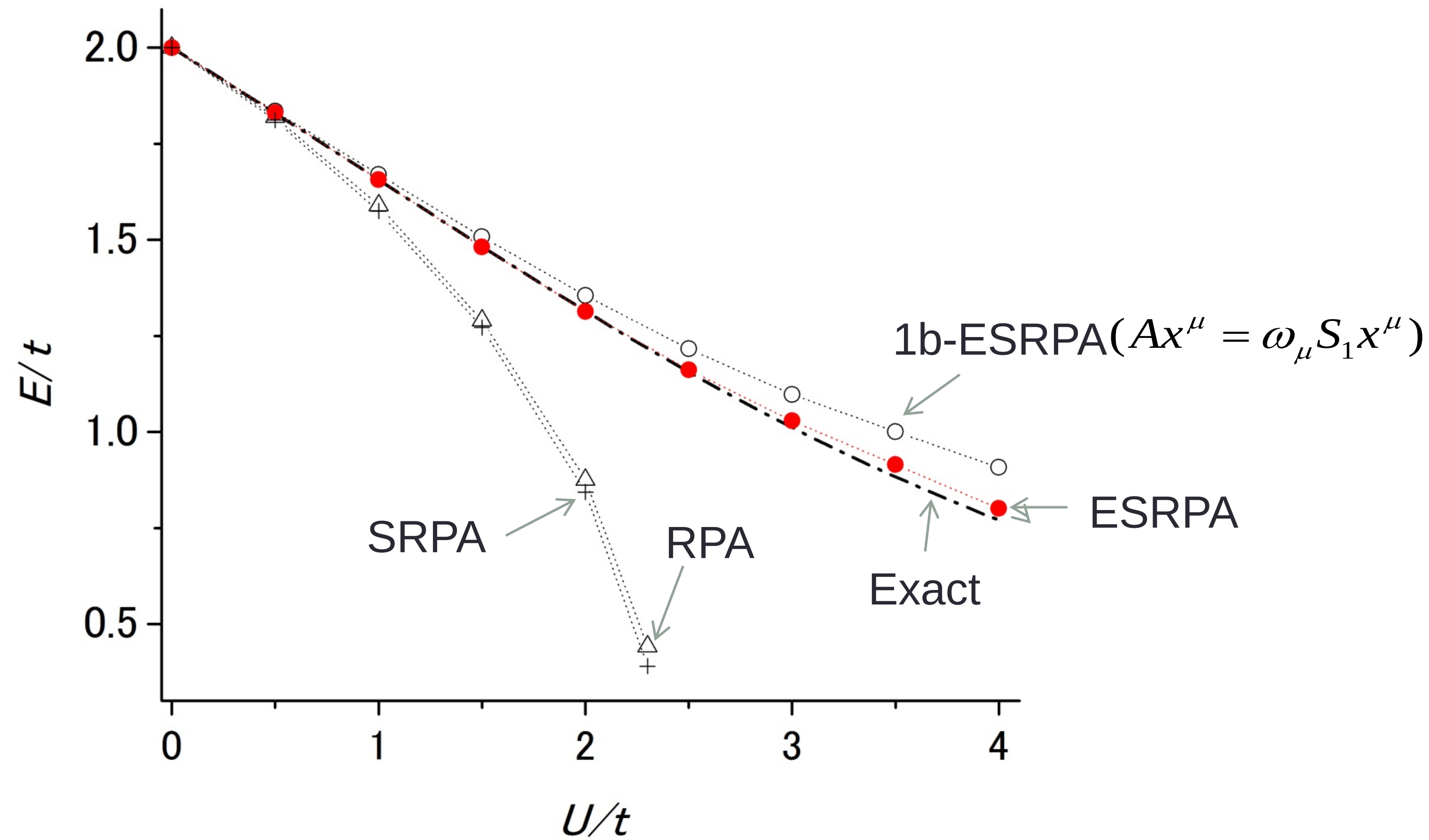


Ground state energy (*N*=6)



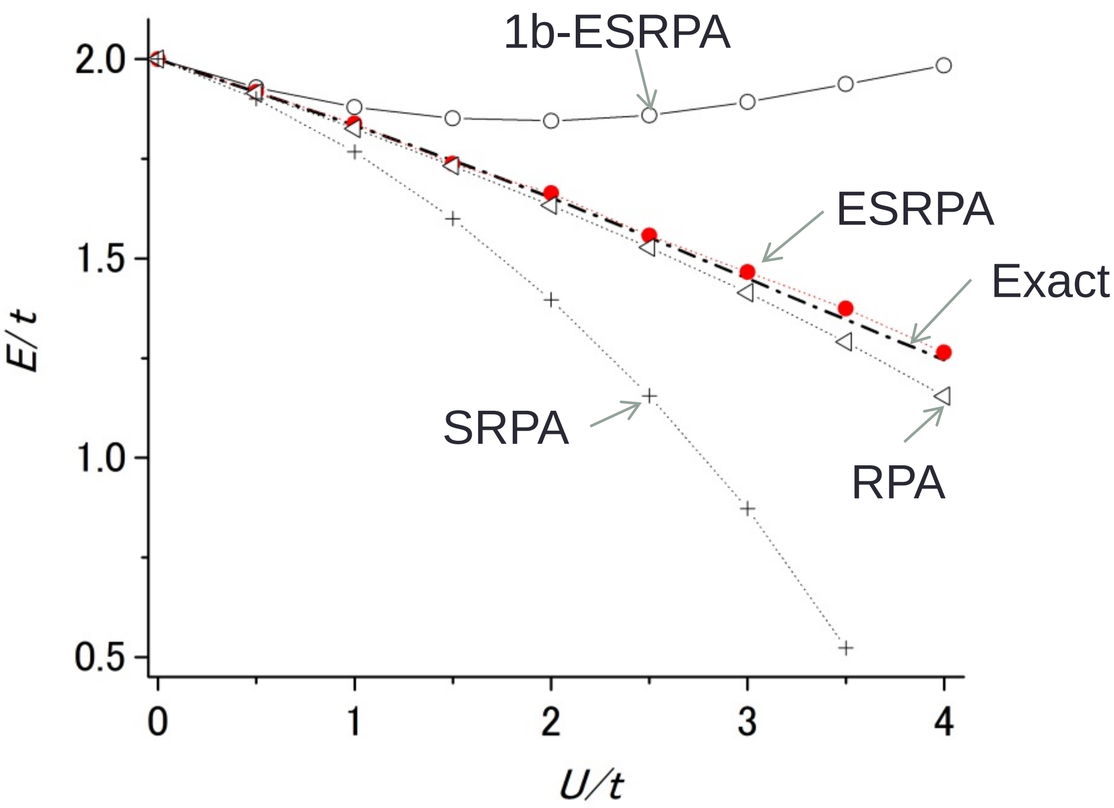
1st excited state (spin mode)

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



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 states

Single-particle states:

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

Residual interaction: simplified Skyrme III

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

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 states

Single-particle states:

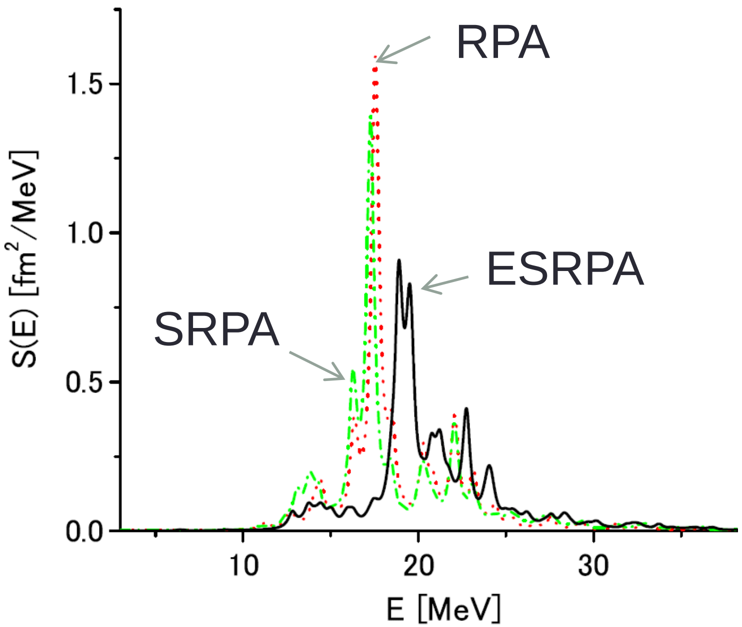
for $x^{\mu}_{\alpha\alpha'} : \varepsilon_{\alpha} \leq 50\ \mathrm{MeV}\ ,\ \ell \leq 11/2$

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

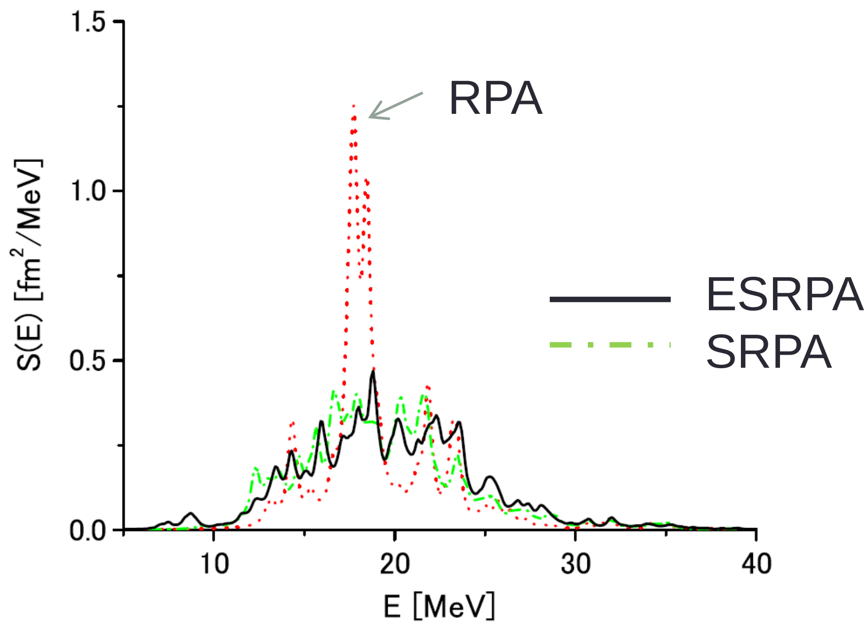
Residual interaction: simplified Skyrme III

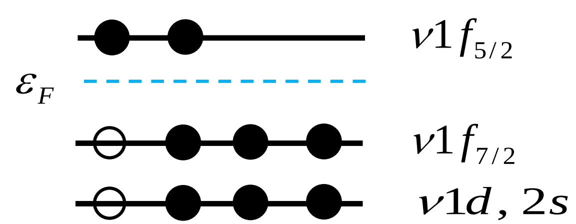
$$v_2 = t_0(1 + x_0 P_{\sigma})\delta^3(\vec{r} - \vec{r}')\ ,\ v_3 = t_3 \delta^3(\vec{r} - \vec{r}')\ \delta^3(\vec{r} - \vec{r}'')$$

^{40}Ca E1

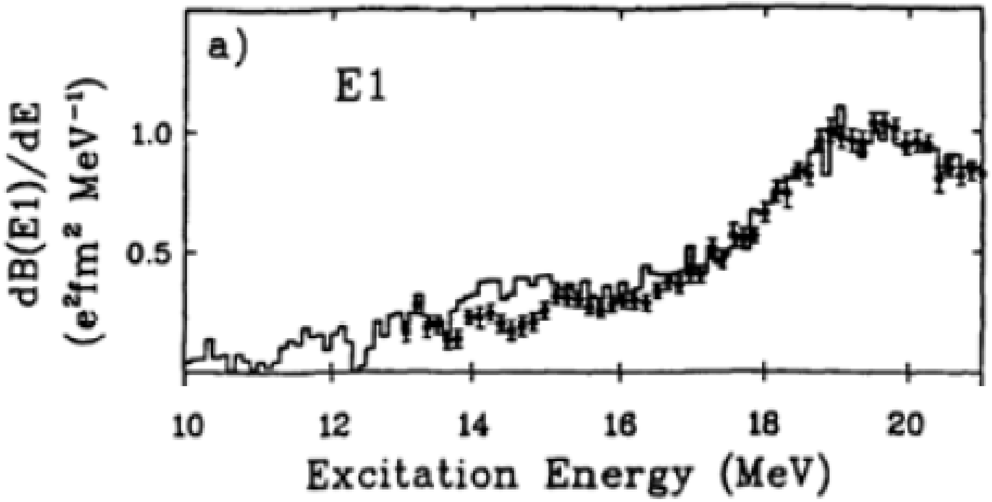


^{48}Ca E1





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

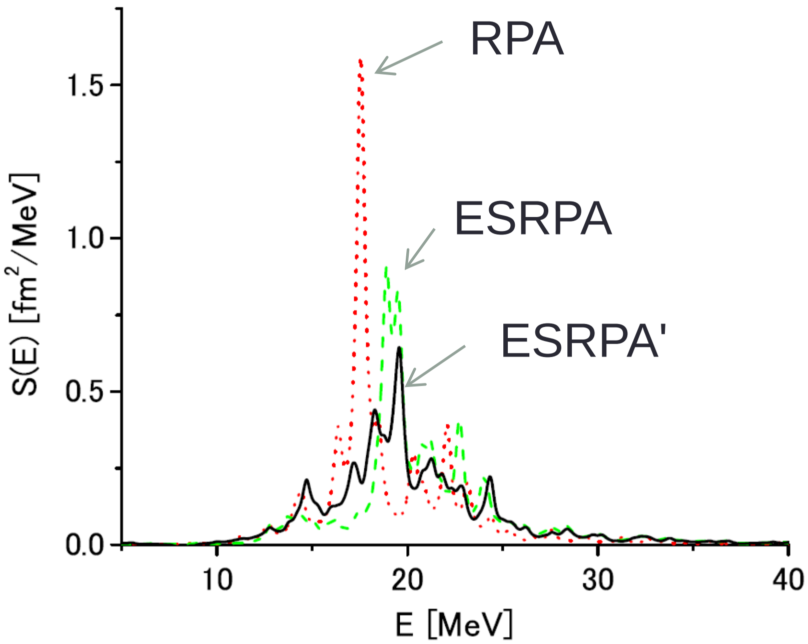


H. Diesner et al. Phys. Rev.Lett. 72, 1994(1994)

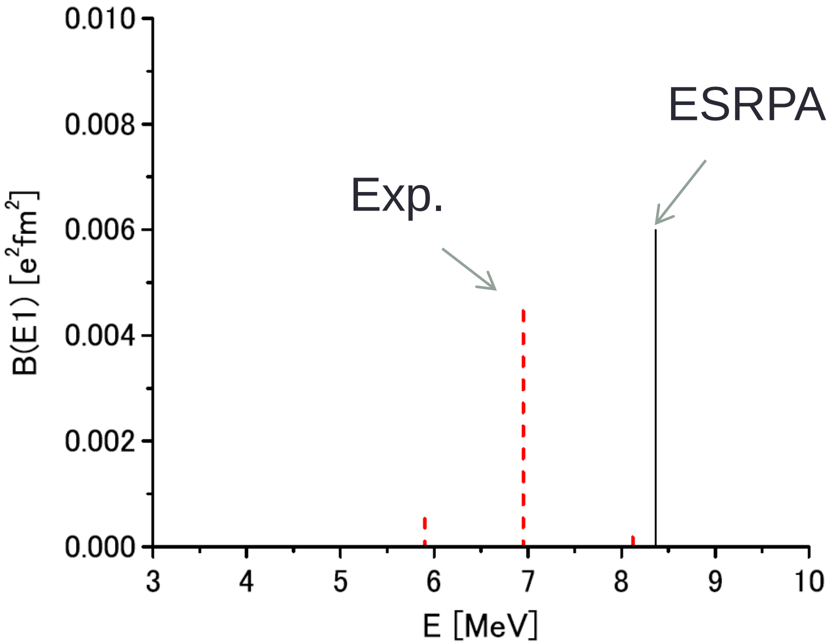
Contributions of 3p-1h and 1p-3h states in ^{40}Ca

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

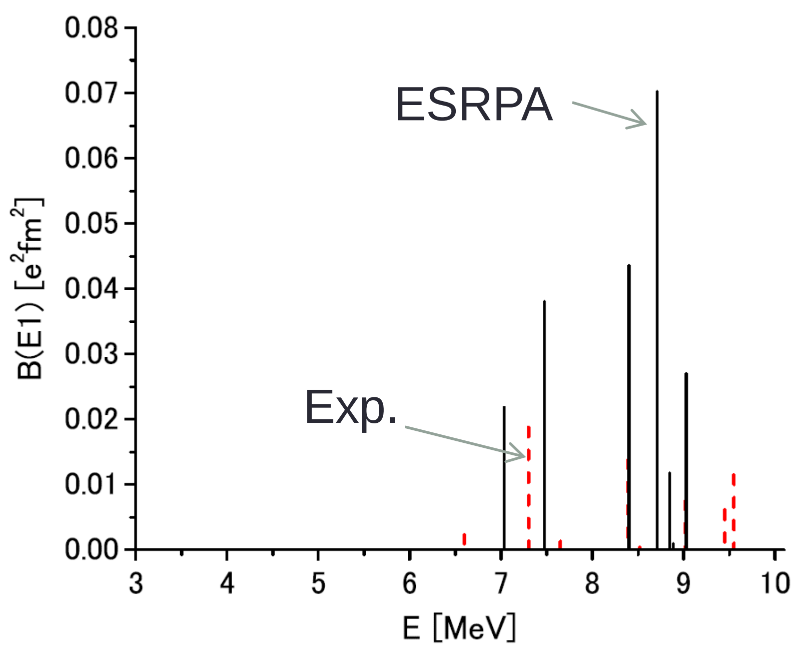
ESRPA' : $X^{\mu}_{pp'hh'} + X^{\mu}_{hh'pp'} + X^{\mu}_{pp'p''h} + X^{\mu}_{phh'h''} + \cdots$



^{40}Ca E1

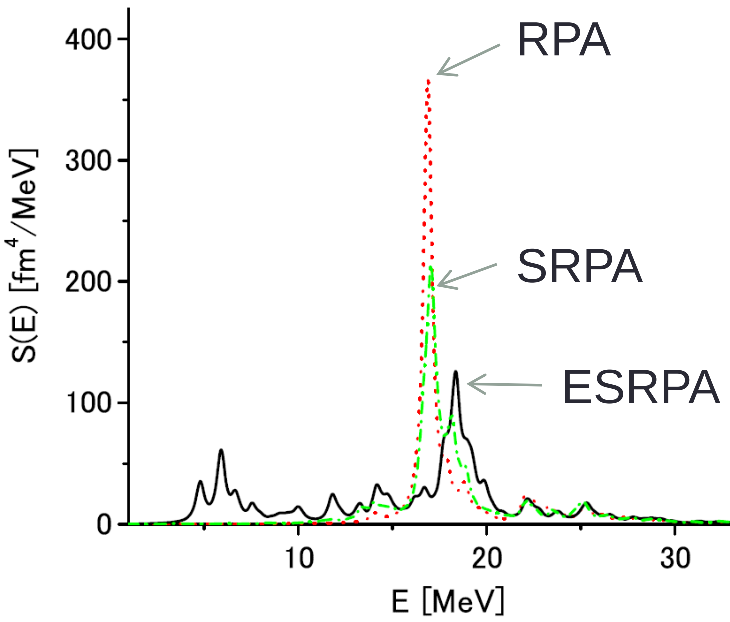


^{48}Ca E1

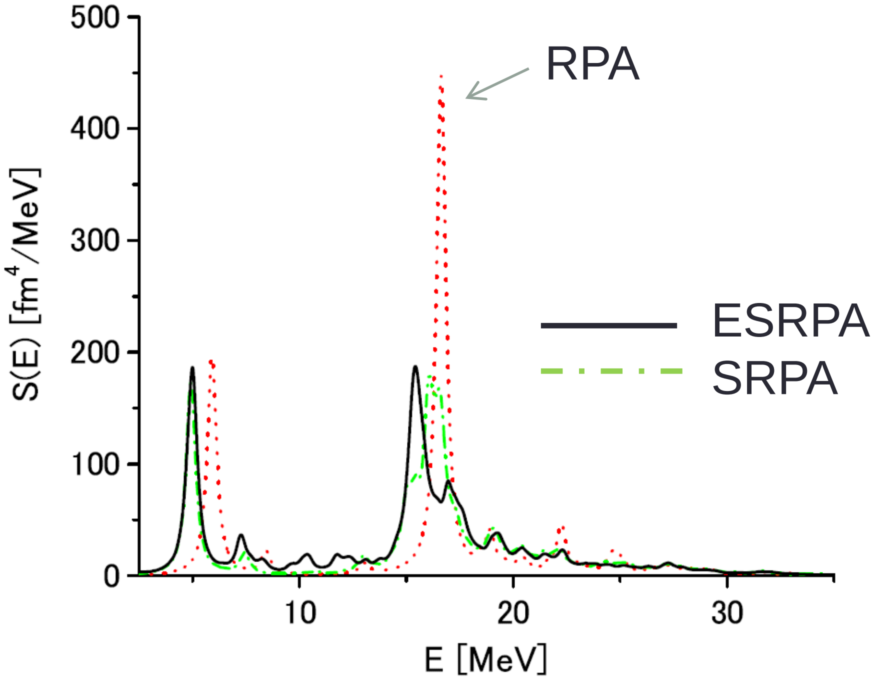


T. Hartmann et al., Phys. Rev. Lett. 85, 274(2000)

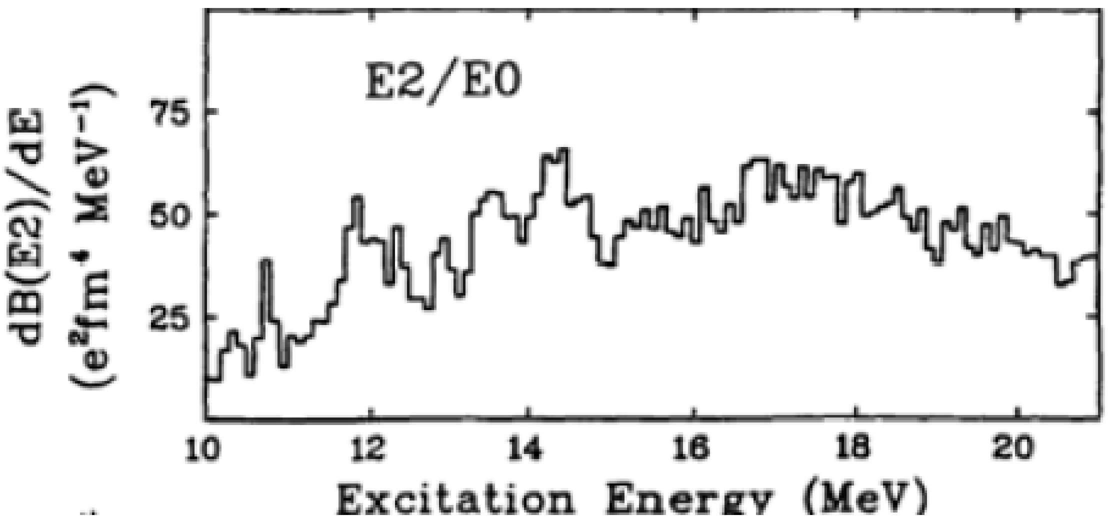
^{40}Ca E2



^{48}Ca E2



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

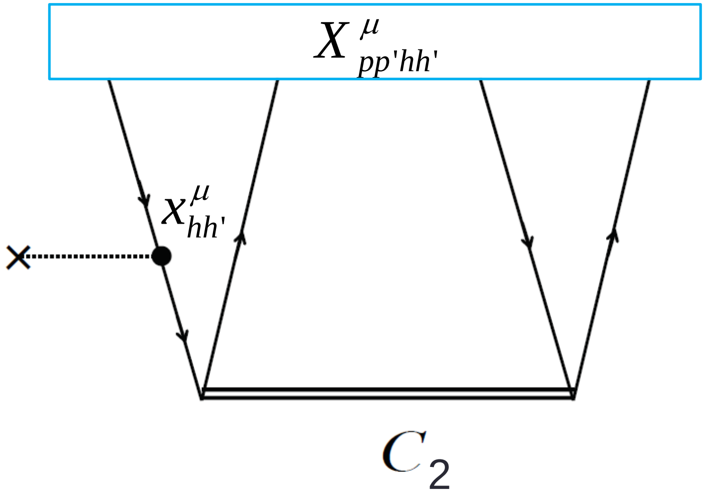


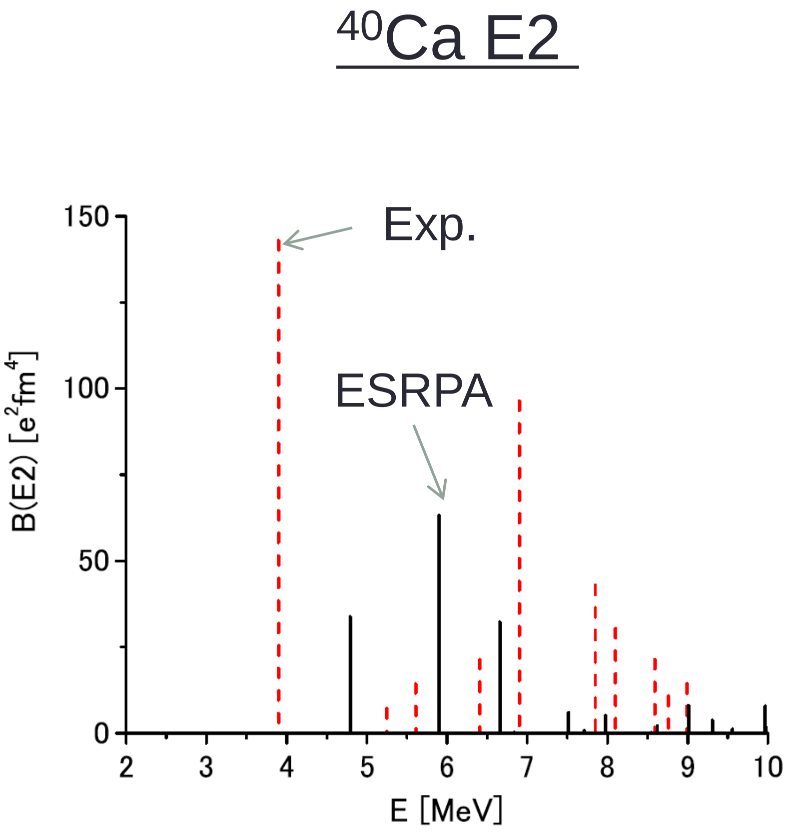
H. Diesner et al. Phys. Rev. Lett. 72, 1994(1994)

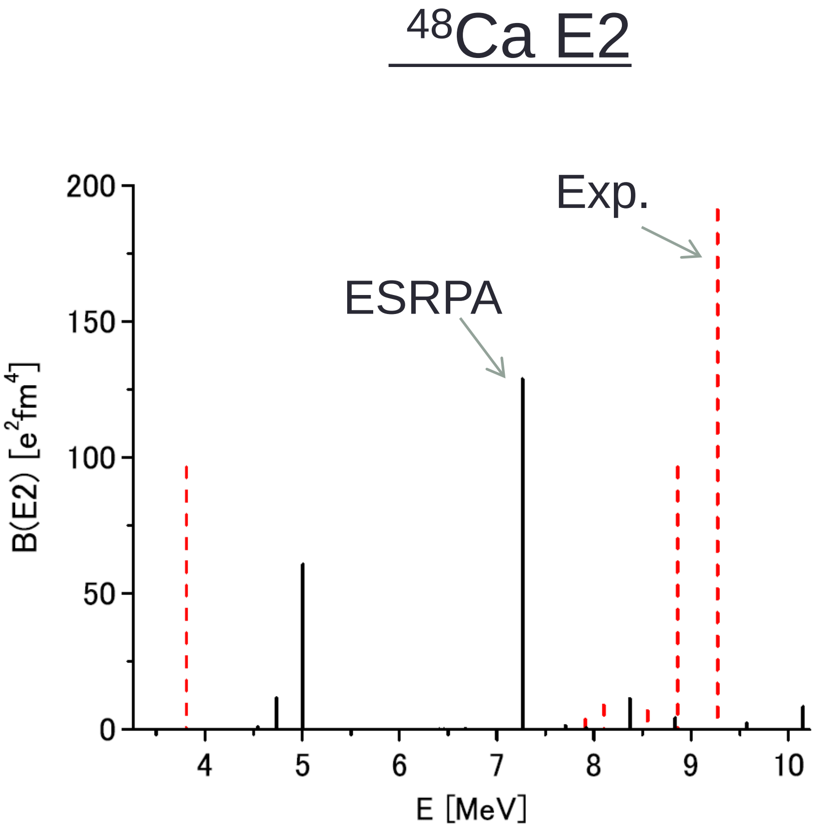
Reasons for strong fragmentation in ^{40}Ca

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

- Contributions of h-h and p-p amplitudes







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

3）Summary

- $C_3 \approx C_2 \times C_2$ gives a better truncation scheme of BBGKY hierarchy for the ground states

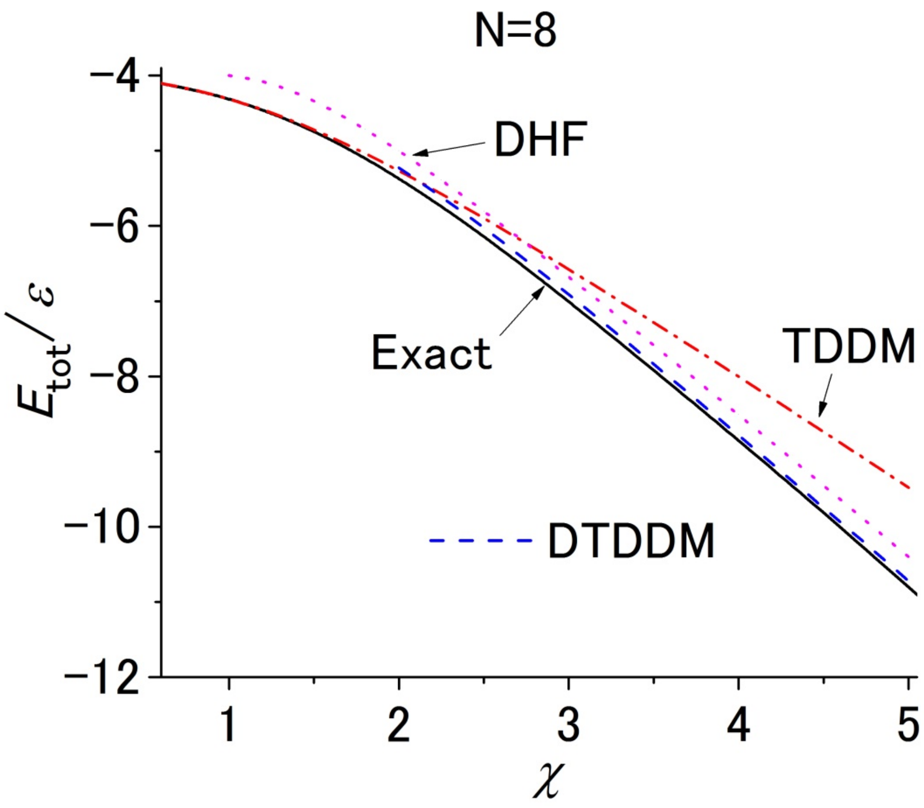
- TDDM+ESRPA works for the excited states

  Self-energy + coupling to $X^{\mu}_{\alpha\beta\alpha'\beta'}$ are important

- Ground-state correlations are important for fragmentation of E1 and E2 in ^{40}Ca and ^{48}Ca

Improvement

TDDM in deformed basis (DTDDM)



Ortho-normalization condition

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

$$\left(x^{\mu *} \;\; X^{\mu *}\right): \text{ left eigen vector}$$