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
3）Relation to coupled-cluster doubles (CCD)
4） 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

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

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

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

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) correlations

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

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

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

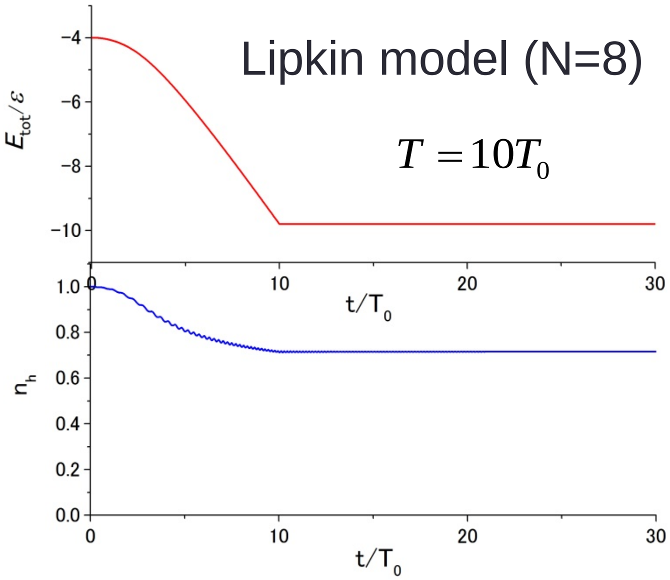
$$C_{p_1p_2h_1p_3p_4h_2} \approx \sum_h z^*_{p_3p_4hh_1} z_{p_1p_2h_2h}, \; C_{p_1h_1h_2p_2h_3h_4} \approx \sum_p z^*_{p_2ph_1h_2} z_{p_1ph_3h_4}$$

Ground state: a stationary solution

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

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

$$Q_\mu^+ = \sum_{\lambda\lambda'} x^\mu_{\lambda\lambda'} a^+_\lambda a_{\lambda'} + \sum_{\lambda_1\lambda_2\lambda_1'\lambda_2'} X^\mu_{\lambda\lambda'} a^+_{\lambda_1} a^+_{\lambda_2} a_{\lambda_2'} a_{\lambda_1'} : \; Q_\mu^+ |\Psi_0\rangle = |\Psi_\mu\rangle , \; Q_\mu |\Psi_0\rangle = 0$$

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

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

↓

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

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

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

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

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

Extended second RPA (ESRPA)

Under HF assumption

$$\begin{pmatrix} n_h = 1 \\ n_p = 0 \\ C_2 = 0 \end{pmatrix} \longrightarrow \text{Second RPA (SRPA)}$$

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

Ortho-normalization condition

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

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

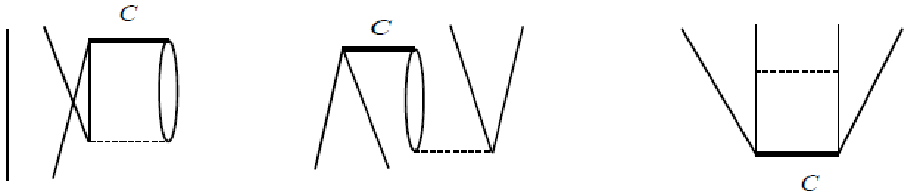
One-body part of ESRPA (1b-ESRPA)

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

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

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

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

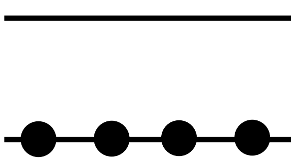


Self-energy

Vertex corrections

3）Applications

Lipkin model



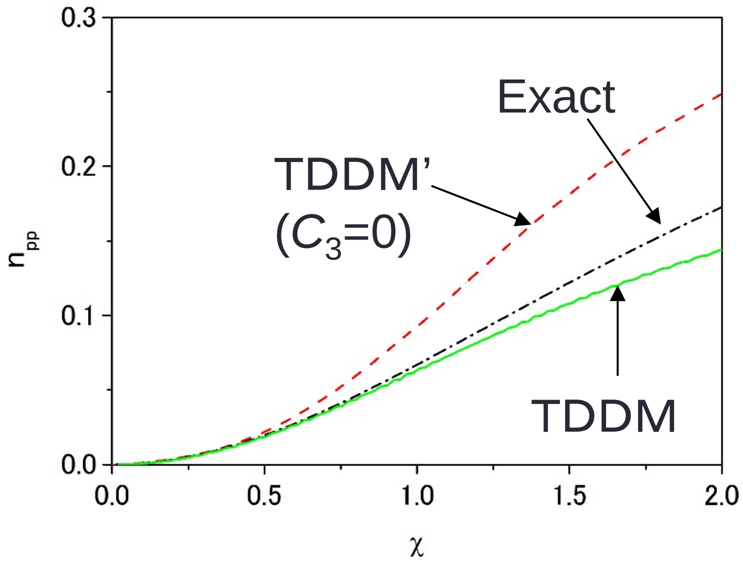
$$H = \varepsilon J_0 + \frac{V}{2}\left(J_+^2 + J_-^2\right)$$

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

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

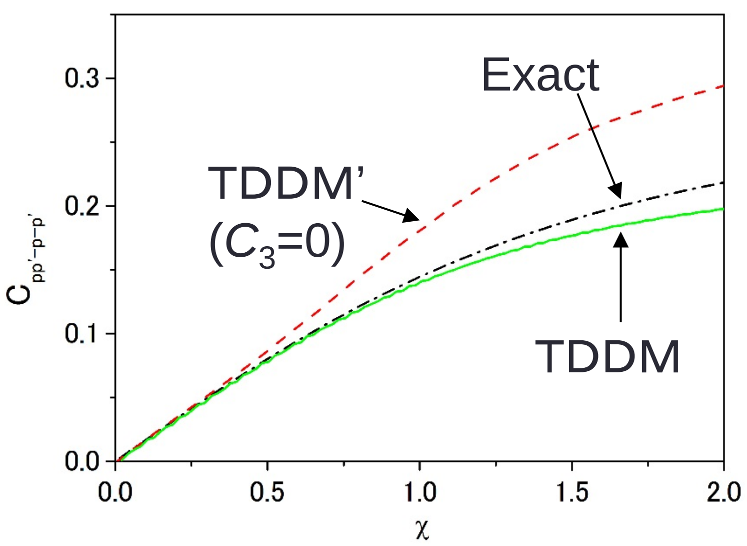
N=4

Occupation probability

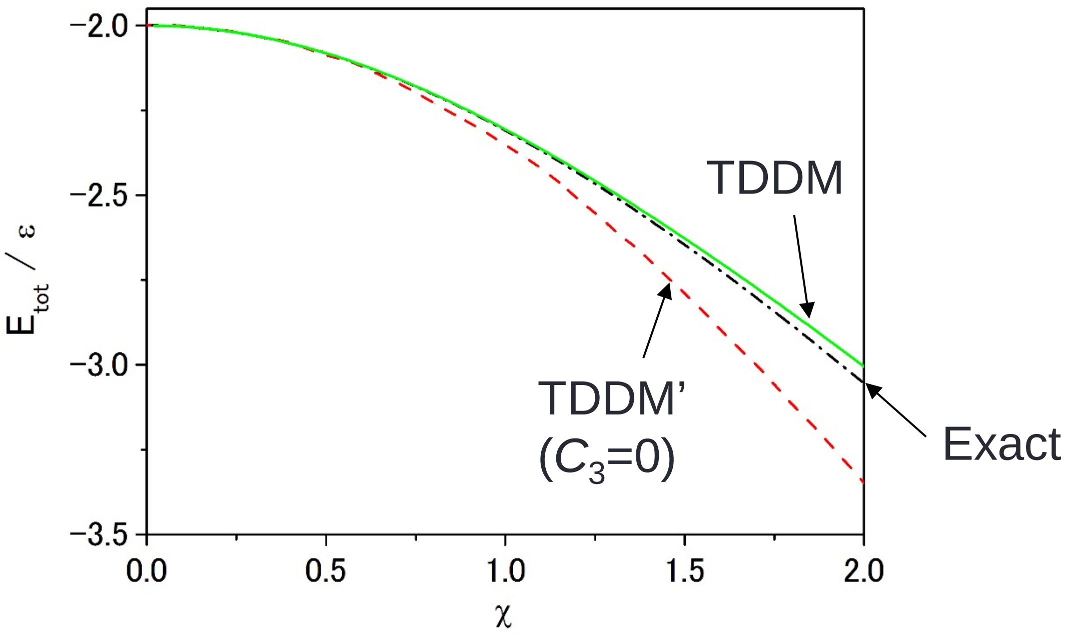


$$\chi = (N-1)\frac{|V|}{\varepsilon}$$

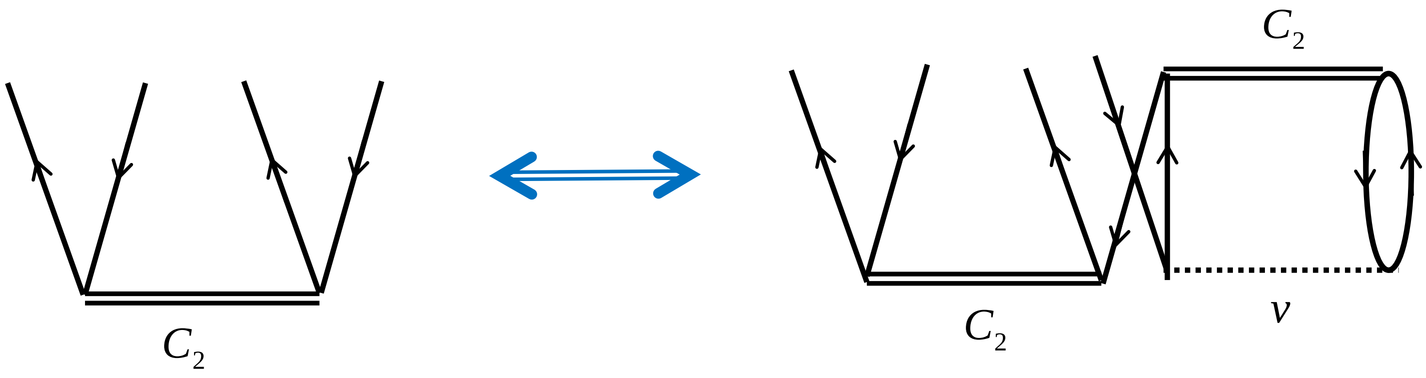
Correlation matrix



Ground state energy N=4



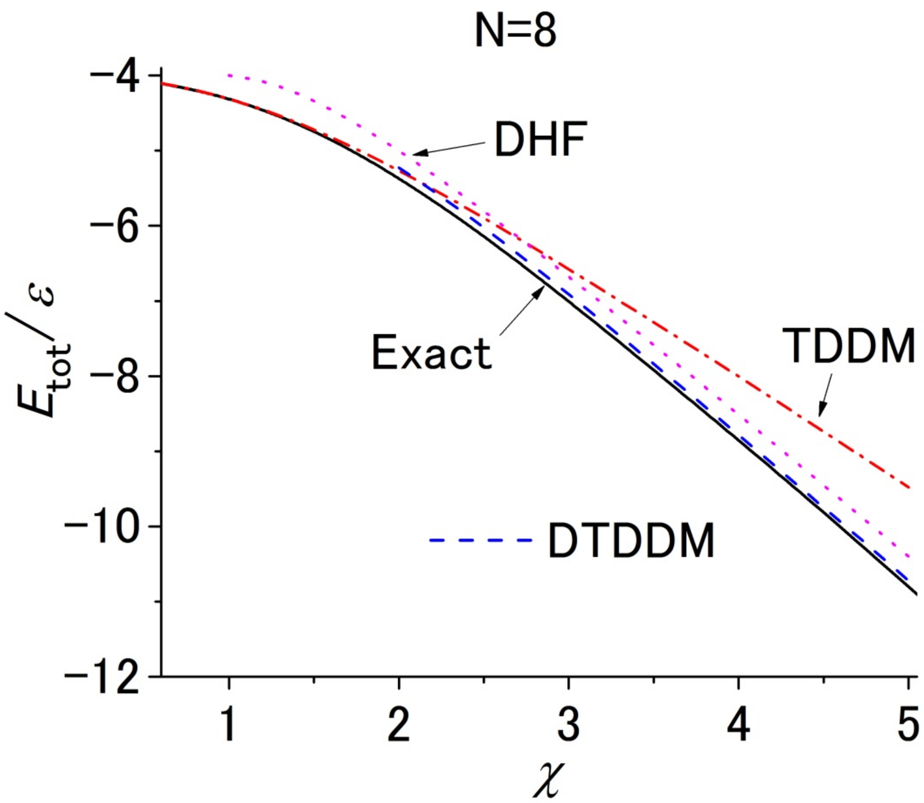
Self-energy contributions from C_3 suppress excess correlations



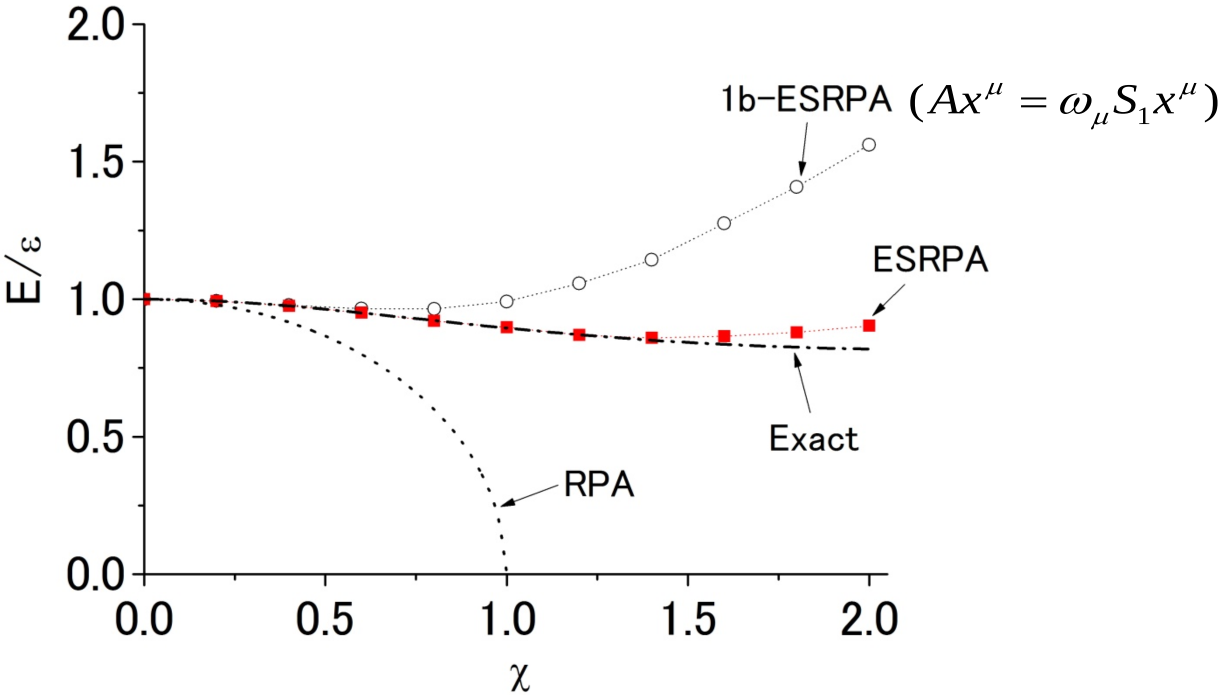
$$C_3 \approx C_2 \times C_2$$

Improvement

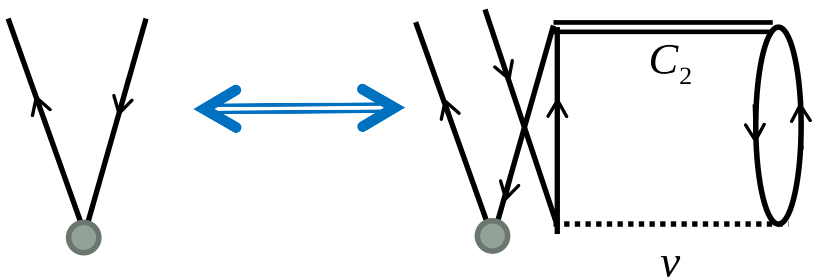
TDDM in deformed basis (DTDDM)



Excited states N=4



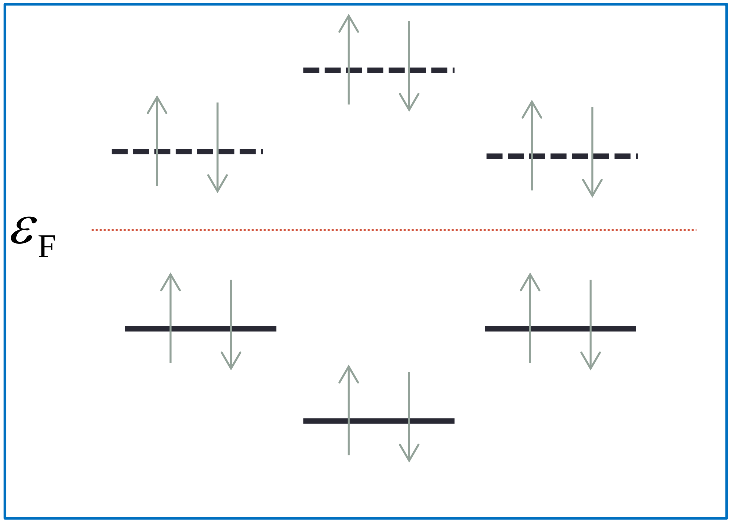
Self-energy contributions
in 1b-ESRPA



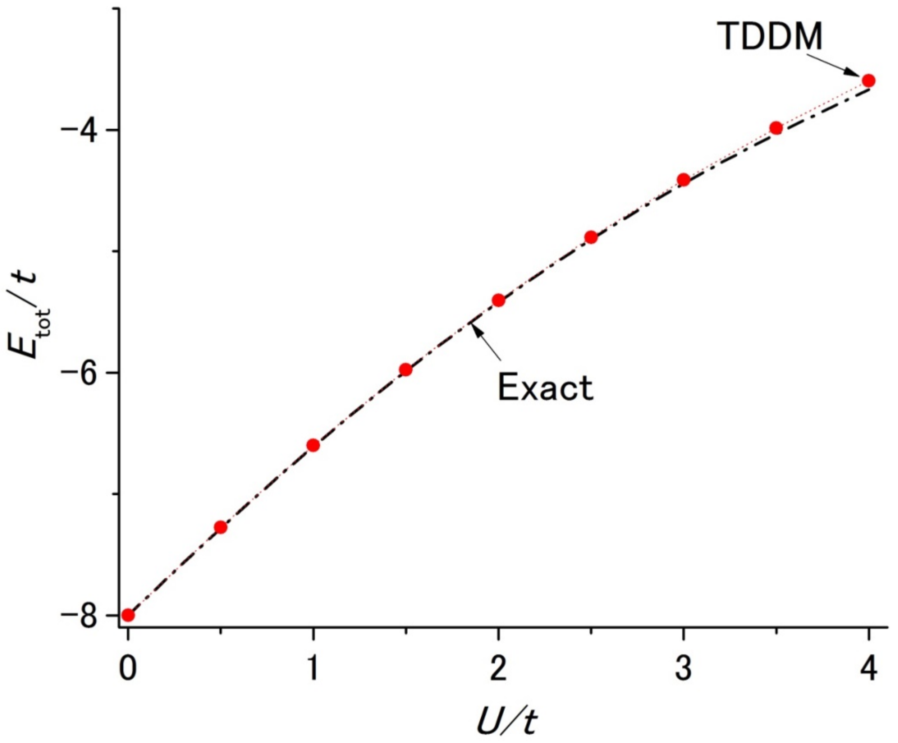
1D-Hubbard model (N=6)

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

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

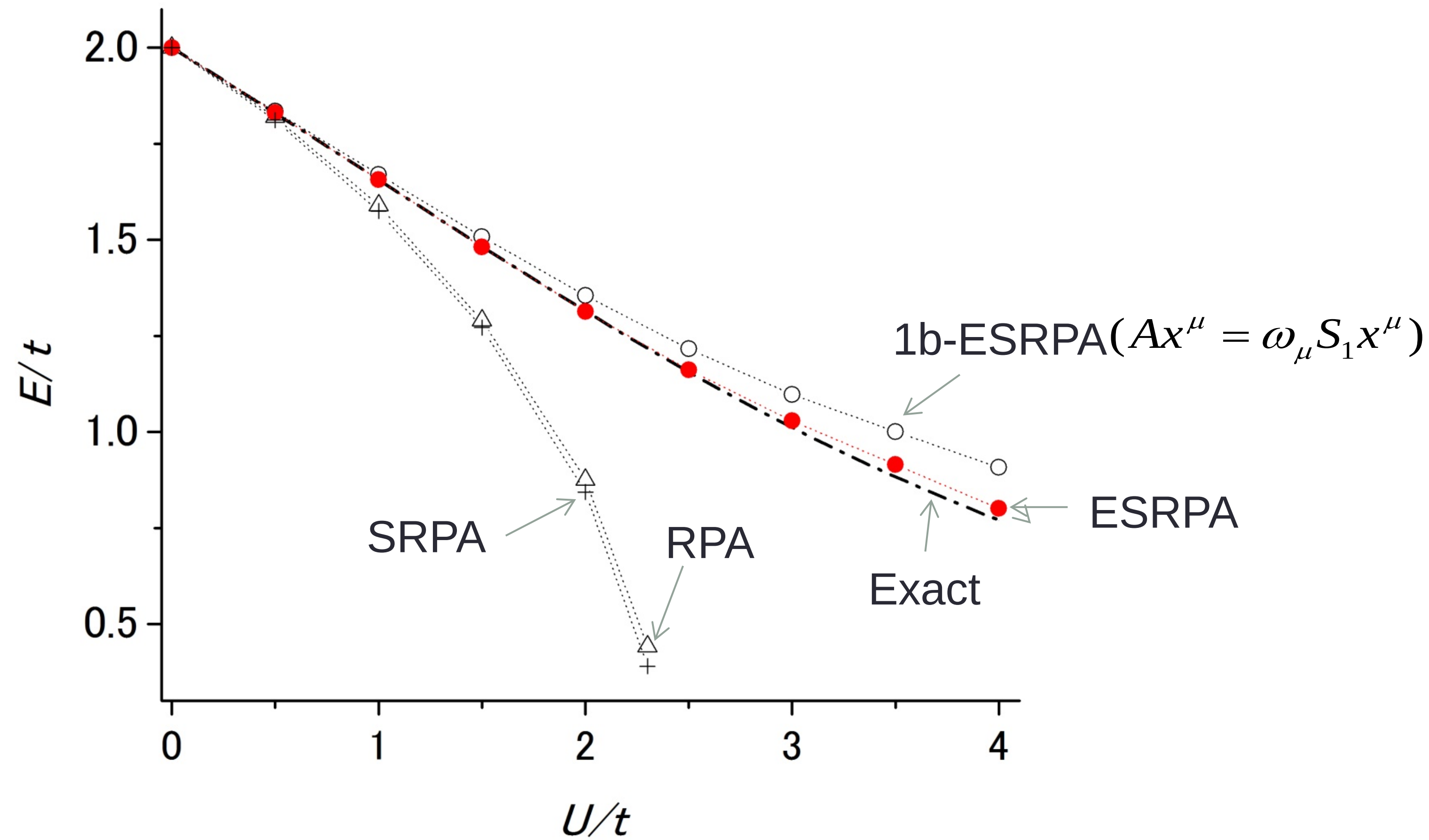


Ground state energy (*N*=6)



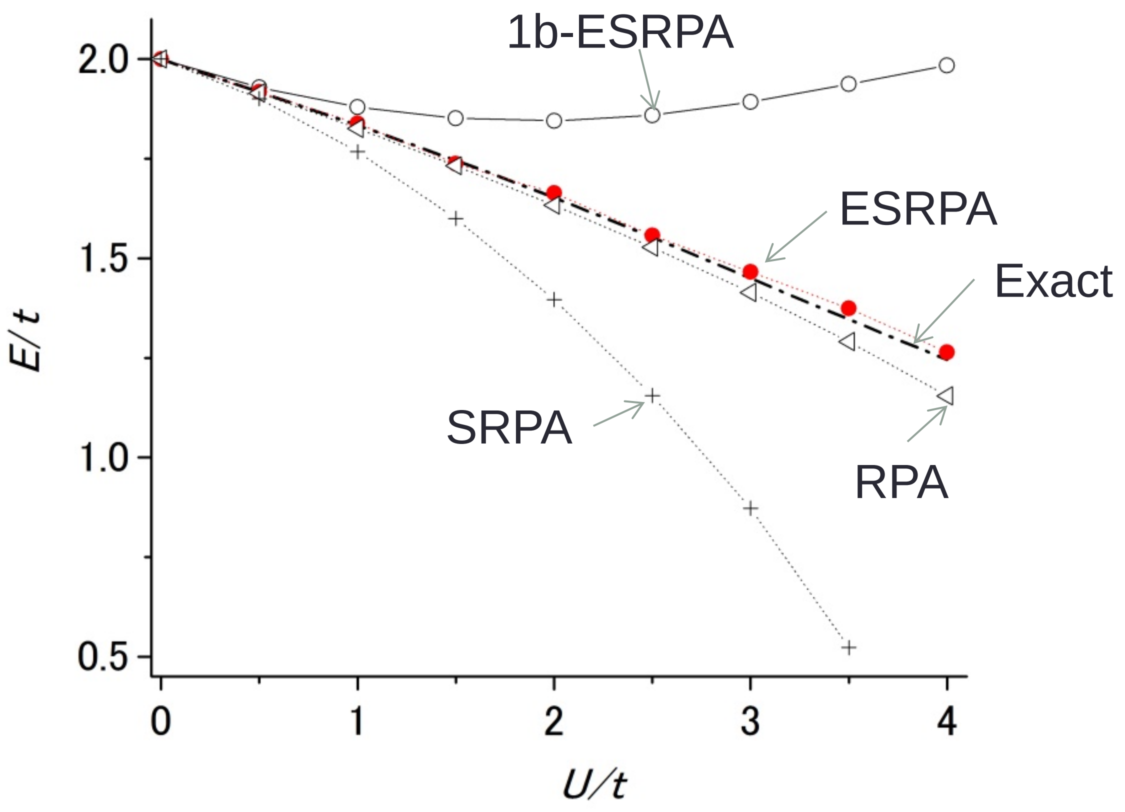
1st excited state (spin mode)

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



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 and coupling to X^{μ} are important

3）Relation of TDDM and CCD

(Tohyama , PTEP 2016, 113D01)

CCD

$$|\Psi_{\mathrm{CCD}}\rangle = e^{T_2}|\mathrm{HF}\rangle, \quad T_2 = \frac{1}{4}\sum_{pp'hh'} t_{pp'hh'} a^+_p a^+_{p'} a_{h'} a_h$$

$$\langle \mathrm{HF}| a^+_h a^+_{h'} a_{p'} a_p e^{-T_2} H e^{T_2} |\mathrm{HF}\rangle = 0$$

TDDM $\left(n_h \approx 1, n_p \approx 0\right)$ CCD

TDDM

$$(\varepsilon_h + \varepsilon_{h'} - \varepsilon_p - \varepsilon_{p'})C_{pp'hh'} = \langle pp'|v|hh'\rangle_A$$
$$+ \sum_{p_1p_2}\langle pp'|v|p_1p_2\rangle C_{p_1p_2hh'} + \sum_{h_1h_2}\langle h_1h_2|v|hh'\rangle C_{pp'h_1h_2}$$
$$+ \sum_{p_1h_1}\left(\langle ph_1|v|h'p_1\rangle_A C_{p'p_1hh_1} - (p \leftrightarrow p', h \leftrightarrow h')\right)$$

$$+ \sum_{h_1h_2}\langle pp'|v|h_1h_2\rangle C_{h_1h_2hh'} + \sum_{p_1p_2}\langle p_1p_2|v|hh'\rangle C_{pp'p_1p_2}$$
$$+ \sum_{p_1h_1}\left(\langle pp_1|v|hh_1\rangle_A C_{h_1p'p_1h'} - (p \leftrightarrow p', h \leftrightarrow h')\right)$$

$$+ \sum_{p_1h_1}\left(\langle pp_1|v|h_1h_2\rangle C_{h_1h_2p_1p_2} C_{p_2p'hh'} - (p \leftrightarrow p', h \leftrightarrow h')\right)$$

CCD

$$(\varepsilon_h + \varepsilon_{h'} - \varepsilon_p - \varepsilon_{p'})t_{pp'hh'} = \langle pp'|v|hh'\rangle_A$$
$$+ \sum_{p_1p_2}\langle pp'|v|p_1p_2\rangle t_{p_1p_2hh'} + \sum_{h_1h_2}\langle h_1h_2|v|hh'\rangle t_{pp'h_1h_2}$$
$$+ \sum_{p_1h_1}\left(\langle ph_1|v|h'p_1\rangle_A t_{p'p_1hh_1} - (p \leftrightarrow p', h \leftrightarrow h')\right)$$

$$+ \sum_{p_1p_2h_1h_2}\langle h_1h_2|v|p_1p_2\rangle_A \Big(t_{p_1p_2hh'}t_{pp'h_1h_2}/4$$
$$+ t_{pp_1hh_1}t_{p'p_2h'h_2} - (p \leftrightarrow p', h \leftrightarrow h')\Big)$$

$$+ \sum_{p_1p_2h_1h_2}\left(\langle h_1h_2|v|p_1p_2\rangle t_{pp_1h_1h_2} t_{p_2p'hh'} - (p \leftrightarrow p', h \leftrightarrow h')\right)$$

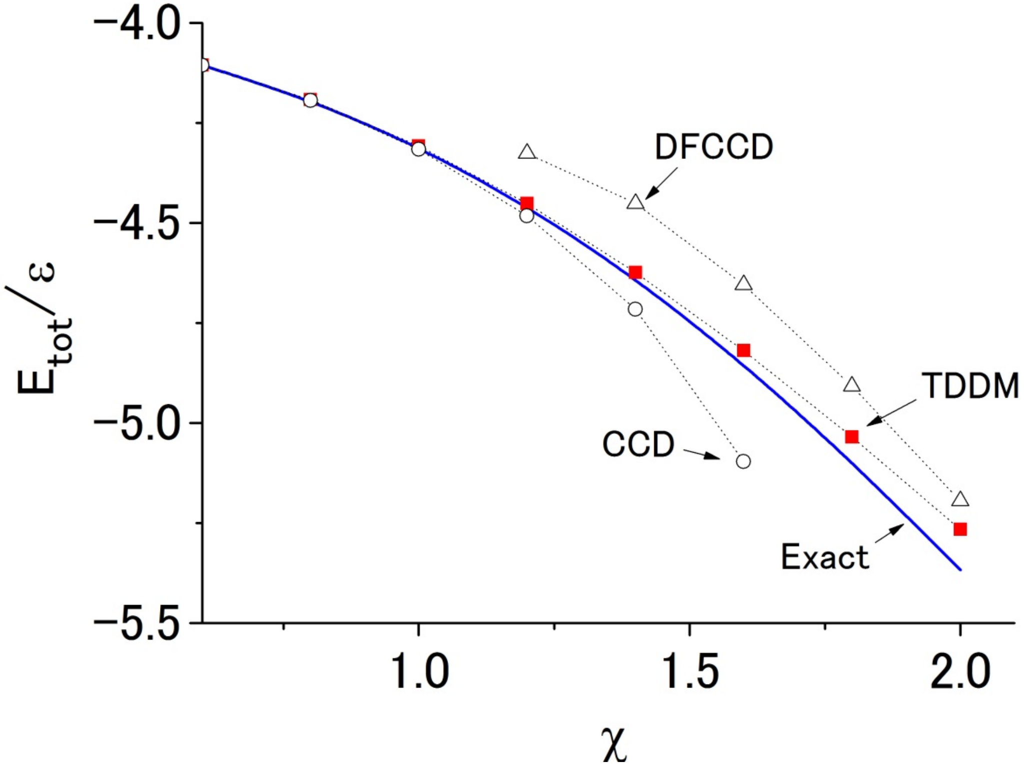
TDDM and CCD have term by term correspondence

$C_{pp'p''p'''}$ is given by $C_{pp'hh'} \times C_{hh'pp'}$

$$C_{pp'p''p'''} \approx \frac{1}{2}\sum_{h_1h_2}\frac{\langle pp'|v|h_1h_2\rangle_A\langle h_1h_2|v|p''p'''\rangle_A}{(\varepsilon_{h_1}+\varepsilon_{h_2}-\varepsilon_p-\varepsilon_{p'})(\varepsilon_{h_1}+\varepsilon_{h_2}-\varepsilon_{p''}-\varepsilon_{p'''})}$$

$$= \frac{1}{2}\sum_{h_1h_2} C_{pp'h_1h_2} C_{h_1h_2p''p'''}$$

Ground state energy (Lipkin model N=8)



Fractional occupation is important in TDDM

2p-2h excitation: $(1-n_p)(1-n_{p'})n_h n_{h'}$

p-p and h-h correlations: $(1-n_p-n_{p'}), \quad (1-n_h-n_{h'})$

p-h correlation: (n_h-n_p)

4) Summary

- $C_3 \approx C_2 \times C_2$ gives a better truncation scheme

- ESRPA gives good description of excited states

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

- TDDM ≈ CCD for $n_h \approx 1, n_p \approx 0$

  TDDM ≠ CCD for a strong interaction