Extended RPA with 3-body ground-state correlations

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- Formulation
- Application to Lipkin model
- Summary

Formulation

TDDM equations

$$\rho(11',t) = \sum_{\alpha\alpha'} n_{\alpha\alpha'}(t)\psi_{\alpha}(1,t)\psi^{*}_{\alpha'}(1',t)$$

$$C_2'(121'2',t) = \rho_2 - A(\rho\rho)$$

$$= \sum_{\alpha\beta\alpha'\beta'} C_{\alpha\beta\alpha'\beta'}(t)\psi_{\alpha}(1,t)\psi_{\beta}(1,t)\psi^{*}_{\alpha'}(1',t)\psi^{*}_{\beta'}(1',t)$$

$$i\hbar\frac{\partial}{\partial t}\psi_{\alpha} = h(\rho)\psi_{\alpha}$$

$$i\hbar\dot{n}_{\alpha\alpha'} = \sum_{\lambda_1\lambda_2\lambda_3}\left(\langle\alpha\lambda_3|v|\lambda_1\lambda_2\rangle C_{\lambda_1\lambda_2\alpha'\lambda_3} - C_{\alpha\lambda_3\lambda_1\lambda_2}\langle\lambda_1\lambda_2|v|\alpha'\lambda_3\rangle\right)$$

$$i\hbar\dot{C}_{\alpha\beta\alpha'\beta'} = B_{\alpha\beta\alpha'\beta'} + P_{\alpha\beta\alpha'\beta'} + H_{\alpha\beta\alpha'\beta'}$$

Extended RPA(ERPA)

Excitation operator

$$Q_\mu^+ = \sum (x_{\lambda\lambda'}^\mu : a_\lambda^+ a_{\lambda'} : + X_{\lambda_1\lambda_2\lambda_1'\lambda_2'}^\mu : a_{\lambda_1}^+ a_{\lambda_2}^+ a_{\lambda_2'} a_{\lambda_1'} :)$$

$$Q_\mu^+ \left| \Psi_0 \right\rangle = \left| \Psi_\mu \right\rangle$$

$$Q_\mu \left| \Psi_0 \right\rangle = 0$$

Equation-of-motion approach

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

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

ERPA equation

$$\begin{pmatrix} A & B \\ C & D \end{pmatrix}\begin{pmatrix} x^{\mu} \\ X^{\mu} \end{pmatrix} = \omega_{\mu}\begin{pmatrix} S_{11} & T_{12} \\ T_{21} & S_{22} \end{pmatrix}\begin{pmatrix} x^{\mu} \\ X^{\mu} \end{pmatrix}$$

$$A(\alpha\alpha':\lambda\lambda') = \langle 0 | [[:a^{+}_{\alpha'}a_{\alpha}:, H], :a^{+}_{\lambda}a_{\lambda'}:] | 0 \rangle$$

$$B(\alpha\alpha':\lambda_1\lambda_2\lambda_1'\lambda_2') = \langle 0 | [[:a^{+}_{\alpha'}a_{\alpha}:, H], :a^{+}_{\lambda_1}a^{+}_{\lambda_2}a_{\lambda_2'}a_{\lambda_1'}:] | 0 \rangle$$

$$C(\alpha\beta\alpha'\beta':\lambda\lambda') = \langle 0 | [[:a^{+}_{\alpha'}a^{+}_{\beta'}a_{\beta}a_{\alpha}:, H], :a^{+}_{\lambda}a_{\lambda'}:] | 0 \rangle$$

$$D(\alpha\beta\alpha'\beta':\lambda_1\lambda_2\lambda_1'\lambda_2') = \langle 0 | [[:a^{+}_{\alpha'}a^{+}_{\beta'}a_{\beta}a_{\alpha}:, H], :a^{+}_{\lambda_1}a^{+}_{\lambda_2}a_{\lambda_2'}a_{\lambda_1'}:] | 0 \rangle$$

$$S_{11}(\alpha\alpha':\lambda\lambda') = \langle 0 | [:a^{+}_{\alpha'}a_{\alpha}:, :a^{+}_{\lambda}a_{\lambda'}:] | 0 \rangle$$

$$T_{12}(\alpha\alpha':\lambda_1\lambda_2\lambda_1'\lambda_2') = \langle 0 | [:a^{+}_{\alpha'}a_{\alpha}:, :a^{+}_{\lambda_1}a^{+}_{\lambda_2}a_{\lambda_2'}a_{\lambda_1'}:] | 0 \rangle$$

$$T_{21}(\alpha\beta\alpha'\beta':\lambda\lambda') = \langle 0 | [:a^{+}_{\alpha'}a^{+}_{\beta'}a_{\beta}a_{\alpha}:, :a^{+}_{\lambda}a_{\lambda'}:] | 0 \rangle$$

$$S_{22}(\alpha\beta\alpha'\beta':\lambda_1\lambda_2\lambda_1'\lambda_2') = \langle 0 | [:a^{+}_{\alpha'}a^{+}_{\beta'}a_{\beta}a_{\alpha}:, :a^{+}_{\lambda_1}a^{+}_{\lambda_2}a_{\lambda_2'}a_{\lambda_1'}:] | 0 \rangle$$

Jacobi 's identity must be fulfilled for ERPA to be Hermitian

$$\langle 0 | [[B,H],A] | 0 \rangle - \langle 0 | [[A,H],B] | 0 \rangle = \langle 0 | [H,[A,B]] | 0 \rangle = 0$$

$$A, B = a_\alpha^+ a_{\alpha'} \text{ or } a_\alpha^+ a_\beta^+ a_{\beta'} a_{\alpha'}$$

This implies

$$\langle 0 | [a_{\alpha'}^+ a_\alpha , H] | 0 \rangle = 0$$

$$\langle 0 | [a_{\alpha'}^+ a_{\beta'}^+ a_\beta a_\alpha , H] | 0 \rangle = 0$$

$$\langle 0 | [a_{\alpha'}^+ a_{\beta'}^+ a_{\gamma'}^+ a_\gamma a_\beta a_\alpha , H] | 0 \rangle = 0$$

One-body part of ERPA

$$Ax^{\mu} = \omega_{\mu} S_{11} x^{\mu}$$

is the same as self-consistent RPA（SCRPA）equation

Ground state |0> is given by

$n_{\alpha\alpha'}$: Occupation matrix

$C_{2\alpha\beta\alpha'\beta'}$: 2-body correlation matrix

$C_{3\alpha\beta\gamma\alpha'\beta'\gamma'}$: 3-body correlation matrix

Stationary conditions

$$\frac{d}{dt} n_{\alpha\alpha'} = F_1 = \langle 0 | [a^+_{\alpha'} a_\alpha, H] | 0 \rangle = 0$$

$$\frac{d}{dt} C_{2\alpha\beta\alpha'\beta'} = F_2 = \langle 0 | [a^+_{\alpha'} a^+_{\beta'} a_\beta a_\alpha, H] | 0 \rangle = 0$$

$$\frac{d}{dt} C_{3\alpha\beta\gamma\alpha'\beta'\gamma'} = F_3 = \langle 0 | [a^+_{\alpha'} a^+_{\beta'} a^+_{\gamma'} a_\gamma a_\beta a_\alpha, H] | 0 \rangle = 0$$

$\longrightarrow$ $n_{\alpha\alpha'}$, $C_{2\alpha\beta\alpha'\beta'}$, $C_{3\alpha\beta\gamma\alpha'\beta'\gamma'}$

Gradient method can be used

$$\begin{pmatrix} \frac{\delta F_1}{\delta n} & \frac{\delta F_1}{\delta C_2} & 0 \\ \frac{\delta F_2}{\delta n} & \frac{\delta F_2}{\delta C_2} & \frac{\delta F_2}{\delta C_3} \\ \frac{\delta F_3}{\delta n} & \frac{\delta F_3}{\delta C_2} & \frac{\delta F_3}{\delta C_3} \end{pmatrix} \begin{pmatrix} \Delta n \\ \Delta C_2 \\ \Delta C_3 \end{pmatrix} = \begin{pmatrix} \Delta F_1 \\ \Delta F_2 \\ \Delta F_3 \end{pmatrix} = \begin{pmatrix} 0 - F_1 \\ 0 - F_2 \\ 0 - F_3 \end{pmatrix}$$

$$\downarrow$$

$$\begin{pmatrix} n(N+1) \\ C_2(N+1) \\ C_3(N+1) \end{pmatrix} = \begin{pmatrix} n(N) \\ C_2(N) \\ C_3(N) \end{pmatrix} - \alpha \begin{pmatrix} \frac{\delta F_1}{\delta n} & \frac{\delta F_1}{\delta C_2} & 0 \\ \frac{\delta F_2}{\delta n} & \frac{\delta F_2}{\delta C_2} & \frac{\delta F_2}{\delta C_3} \\ \frac{\delta F_3}{\delta n} & \frac{\delta F_3}{\delta C_2} & \frac{\delta F_3}{\delta C_3} \end{pmatrix}^{-1} \begin{pmatrix} F_1(N) \\ F_2(N) \\ F_3(N) \end{pmatrix}$$

N : Iteration step

Relation to the variational principle

$$|\Phi'\rangle = e^{iF}|0\rangle$$

$$F = F^{+} = \sum (f_{\alpha\alpha'} a^{+}_{\alpha} a_{\alpha'} + f_{\alpha\beta\alpha'\beta'} a^{+}_{\alpha} a^{+}_{\beta} a_{\beta'} a_{\alpha'})$$

$$E = \langle 0|e^{-iF} H e^{iF}|0\rangle \approx E_0 + i\sum \left(\langle 0|[H, a^{+}_{\alpha} a_{\alpha'}]|0\rangle, \langle 0|[H, a^{+}_{\alpha} a^{+}_{\beta} a_{\beta'} a_{\alpha'}]|0\rangle\right) \begin{pmatrix} f_{\alpha\alpha'} \\ f_{\alpha\beta\alpha'\beta'} \end{pmatrix}$$

$$\frac{\delta E}{\delta f_{\alpha\alpha'}} = i\langle 0|[H, a^{+}_{\alpha} a_{\alpha'}]|0\rangle = 0$$

$$\frac{\delta E}{\delta f_{\alpha\beta\alpha'\beta'}} = i\langle 0|[H, a^{+}_{\alpha} a^{+}_{\beta} a_{\beta'} a_{\alpha'}]|0\rangle = 0$$

Expressions for F_1, F_2 and F_3

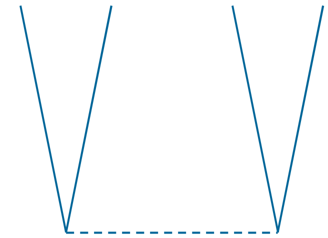
$$F_{1\alpha\alpha'}(n, C_2) = (\varepsilon_\alpha - \varepsilon_{\alpha'}) n_{\alpha\alpha'} + \sum_{\lambda_1\lambda_2\lambda_3} \left\{ \langle \alpha\lambda_3 | v | \lambda_1\lambda_2 \rangle C_{2\lambda_1\lambda_2\alpha'\lambda_3} - C_{2\alpha\lambda_3\lambda_1\lambda_2} \langle \lambda_1\lambda_2 | v | \alpha'\lambda_3 \rangle \right\}$$

$$F_{2\alpha\beta\alpha'\beta'}(n, C_2, C_3) = (\varepsilon_\alpha + \varepsilon_\beta - \varepsilon_{\alpha'} - \varepsilon_{\beta'}) C_{2\alpha\beta\alpha'\beta'} + B_{\alpha\beta\alpha'\beta'} + P_{\alpha\beta\alpha'\beta'} + H_{\alpha\beta\alpha'\beta'} + T_{\alpha\beta\alpha'\beta'}$$

$$F_{3\alpha\beta\gamma\alpha'\beta'\gamma'}(n, C_2, C_3) = (\varepsilon_\alpha + \varepsilon_\beta + \varepsilon_\gamma - \varepsilon_{\alpha'} - \varepsilon_{\beta'} - \varepsilon_{\gamma'}) C_{3\alpha\beta\gamma\alpha'\beta'\gamma'} + \ldots\ldots$$

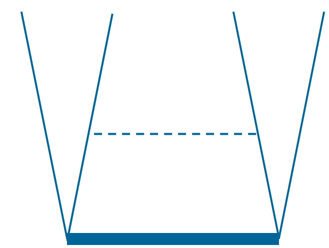
B, *P*, *H* terms

$$B_{\alpha\beta\alpha'\beta'} = \sum_{\lambda_1\lambda_2\lambda_3\lambda_4} \langle \lambda_1\lambda_2 | v | \lambda_3\lambda_4 \rangle_A$$
$$\times [(\delta_{\alpha\lambda_1} - n_{\alpha\lambda_1})(\delta_{\beta\lambda_2} - n_{\beta\lambda_2}) n_{\lambda_3\alpha'} n_{\lambda_4\beta'}$$
$$- (\alpha, \beta \Leftrightarrow \alpha', \beta')]$$



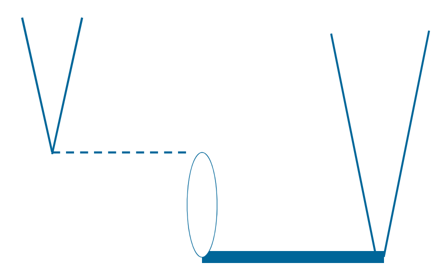
2p-2h excitations

$$P_{\alpha\beta\alpha'\beta'} = \sum_{\lambda_1\lambda_2\lambda_3\lambda_4} \langle \lambda_1\lambda_2 | v | \lambda_3\lambda_4 \rangle$$
$$\times [(\delta_{\alpha\lambda_1}\delta_{\beta\lambda_2} - \delta_{\alpha\lambda_1} n_{\beta\lambda_2} - \delta_{\beta\lambda_2} n_{\alpha\lambda_1}) C_{2\lambda_3\lambda_4\alpha'\beta'}$$
$$- (\alpha, \beta \Leftrightarrow \alpha', \beta')]$$



p-p and h-h correlations

$$H_{\alpha\beta\alpha'\beta'} = \sum_{\lambda_1\lambda_2\lambda_3\lambda_4} \langle \lambda_1\lambda_2 | v | \lambda_3\lambda_4 \rangle_A$$
$$\times [(\delta_{\alpha\lambda_1} n_{\lambda_3\alpha'} - \delta_{\lambda_3\alpha'} n_{\alpha\lambda_1}) C_{2\lambda_4\beta\lambda_2\beta'} + (\alpha, \beta \Leftrightarrow \alpha', \beta')$$
$$- (\delta_{\beta\lambda_1} n_{\lambda_3\alpha'} - \delta_{\lambda_3\alpha'} n_{\beta\lambda_1}) C_{2\lambda_4\alpha\lambda_2\beta'} - (\alpha, \beta \Leftrightarrow \alpha', \beta')]$$



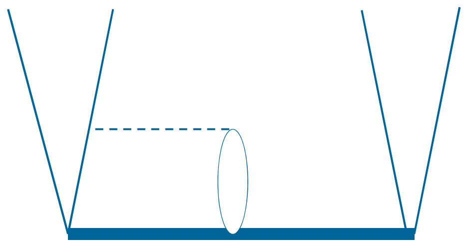
P-h correlations

T term

$$T_{\alpha\beta\alpha'\beta'} = \sum_{\lambda_1\lambda_2\lambda_3\lambda_4} \langle \lambda_1\lambda_2 | v | \lambda_3\lambda_4 \rangle$$

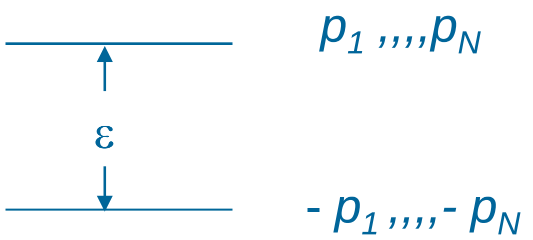
$$\times [\delta_{\alpha\lambda_1} C_{3\lambda_3\lambda_4\beta\alpha'\lambda_2\beta'} + \delta_{\beta\lambda_2} C_{3\lambda_4\lambda_3\alpha\beta'\lambda_1\alpha'}$$

$$- \delta_{\alpha'\lambda_3} C_{3\alpha\lambda_4\beta\lambda_1\lambda_2\beta'} - \delta_{\beta'\lambda_4} C_{3\alpha\lambda_3\beta\lambda_1\lambda_2\alpha'}]$$



interferes with p-p and p-h correlations

Application to Lipkin model

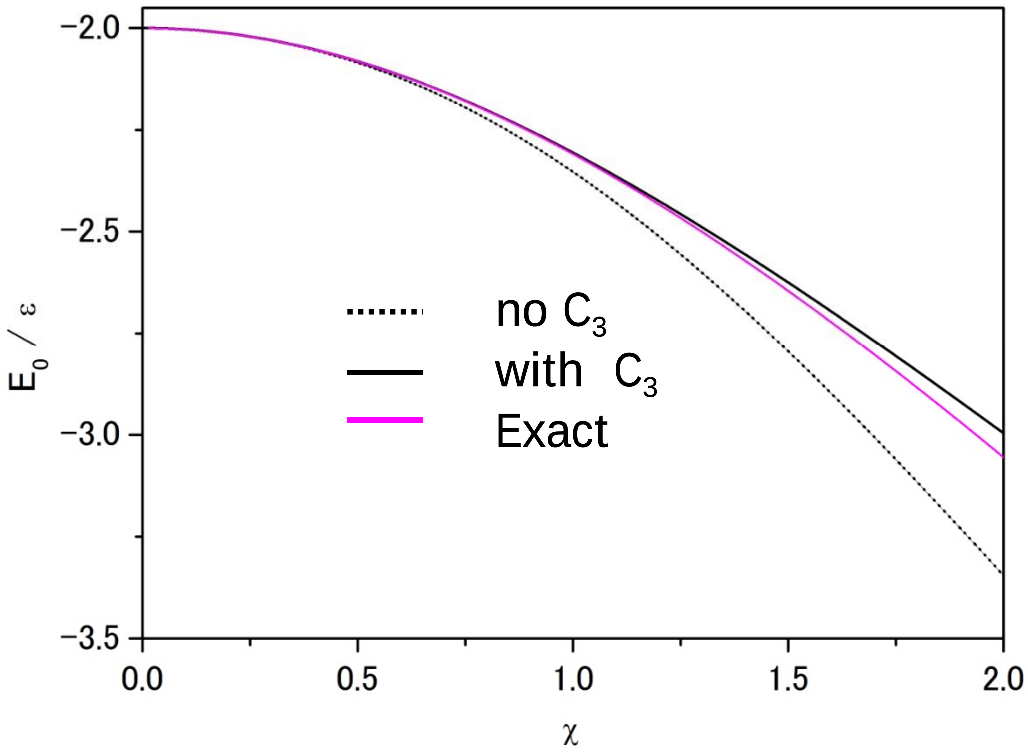


$$H = \varepsilon J_z + \frac{1}{2} V (J_+^2 + J_-^2)$$

$$J_z = \frac{1}{2} \sum_p (a_p^+ a_p - a_{-p}^+ a_{-p}), \quad J_+ = J_-^+ = \sum_p a_p^+ a_{-p}$$

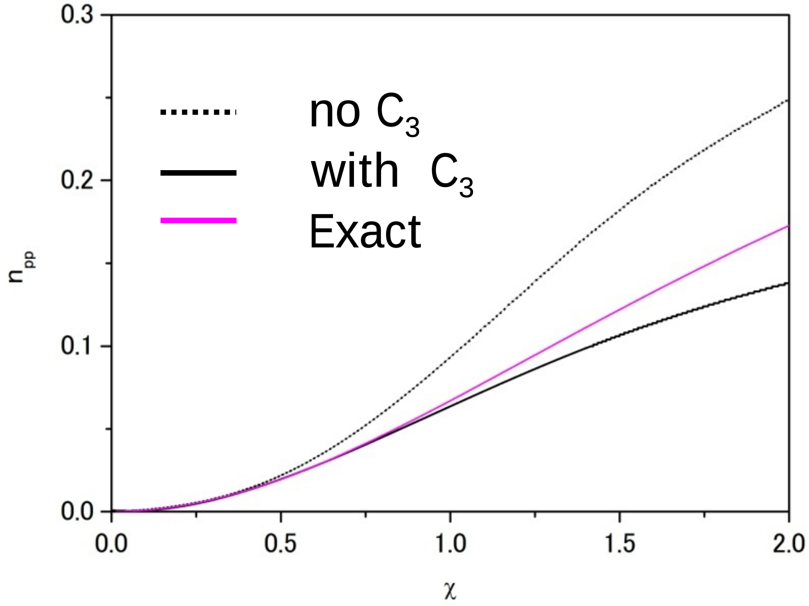
$$[J_+, J_-] = 2 J_z , \quad [J_z, J_\pm] = \pm J_\pm$$

Ground-state energy（N=4）



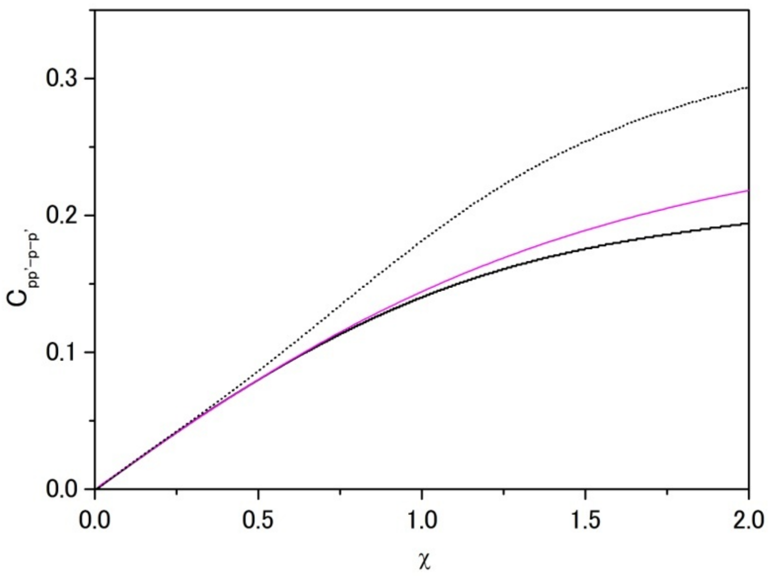
$\chi=(N-1)V/\varepsilon$

n_{pp}



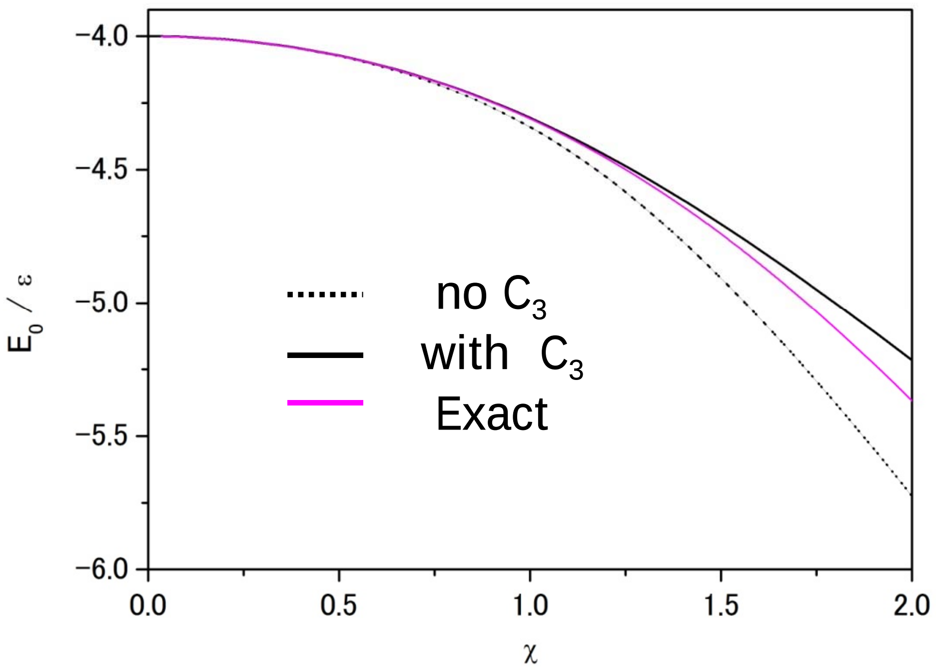
0.3
0.2
0.1
0.0
no C3
with C3
Exact
n_pp
0.0
0.5
1.0
1.5
2.0
χ

$C_{pp'-p-p'}$



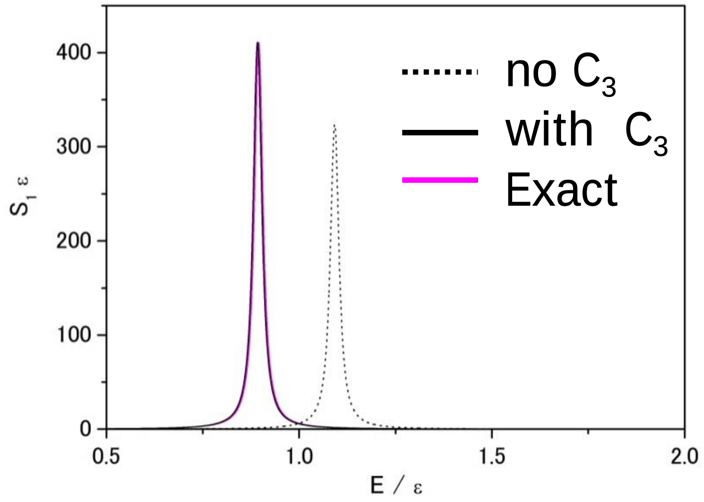
0.3
0.2
0.1
0.0
C_pp'-p-p'
0.0
0.5
1.0
1.5
2.0
χ

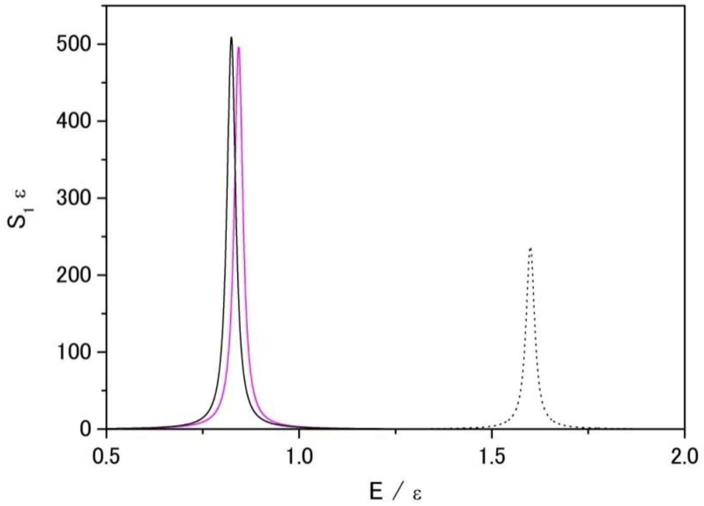
Ground-state energy (N=8)



One-phonon state (N=4)

$$Q_\mu^+ = J_+ + J_-$$



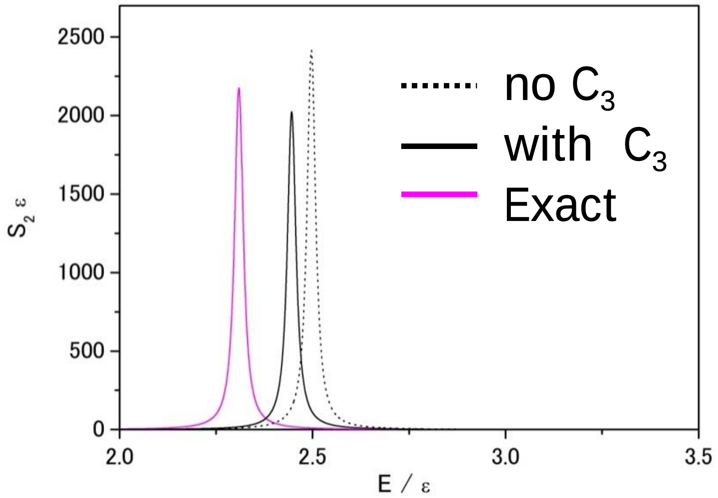


$\chi=(N-1)V/\varepsilon=1$

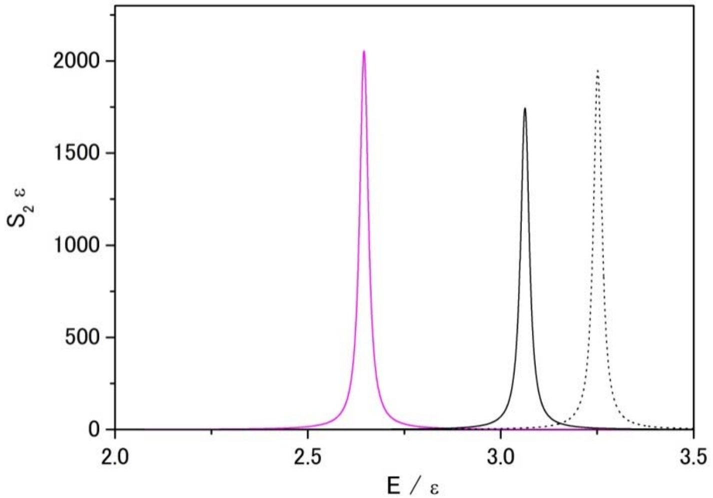
$\chi=1.5$

2 phonon state (N=4)

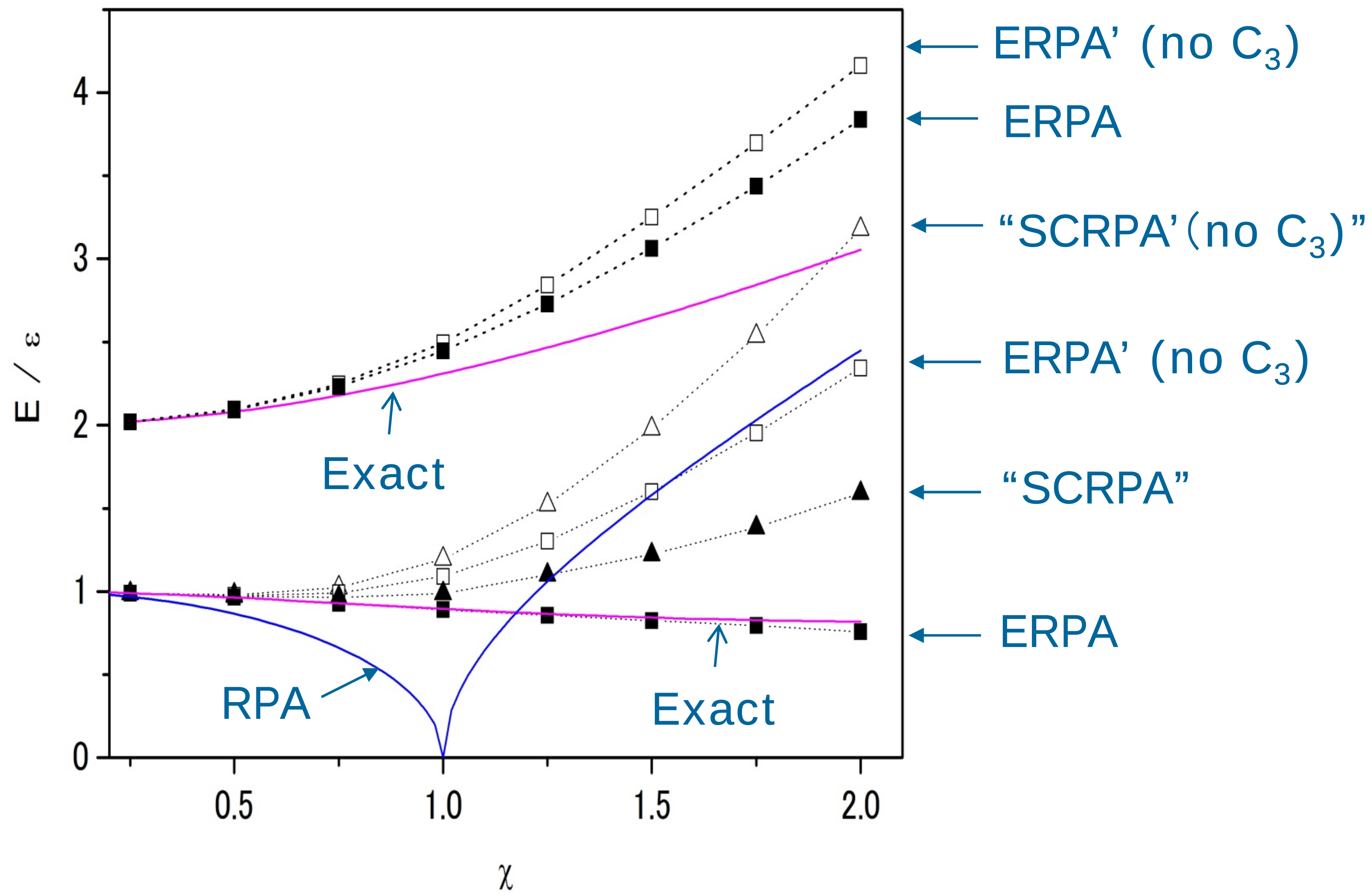
$$Q_{\mu}^{+} = (J_{+} + J_{-})^{2}$$



$\chi = 1$



$\chi = 1.5$



E / ε
4
3
2
1
0
0.5
1.0
1.5
2.0
χ
Exact
RPA
Exact
ERPA' (no C3)
ERPA
"SCRPA'(no C3)"
ERPA' (no C3)
"SCRPA"
ERPA

Summary

- 3-body g.s. correlations guarantee Hermiticity
- 3-body g.s. correlations drastically improve the results for the Lipkin model