Adiabatic approach to large-amplitude collective motion with the higher-order collective-coordinate operator

KS, Prog. Theor. Exp. Phys. 2018, 103D01

Koichi Sato (Osaka City Univ.)

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Adiabatic Self-consistent Collective Coordinate (ASCC)Method

Matsuo, Nakatsukasa, and Matsuyanagi, PTP 103(2000), 959.

⇩

Adiabatic approx. to SCC method T. Marumori, T. Maskawa, F. Sakata and A. Kuriyama, PTP **64** (1980), 1294.

- One can extract the collective degree(s) of freedom the system itself chooses

Invariance principle of Schroedinger eq.

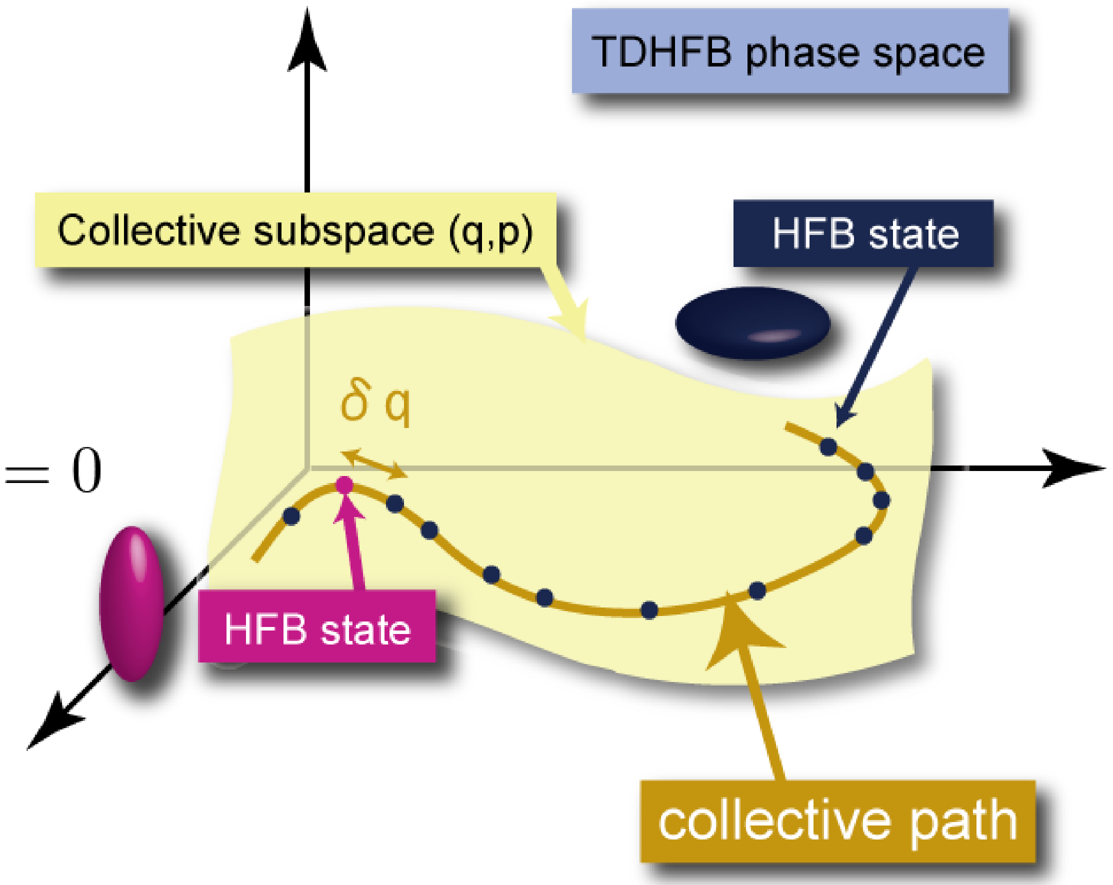
$$\delta\langle\phi(q,p,\varphi,n)|i\partial_t - \hat{H}|\phi(q,p,\varphi,n)\rangle = 0$$

Adiabatic expansion

(in powers of coll. mom. p)

↓

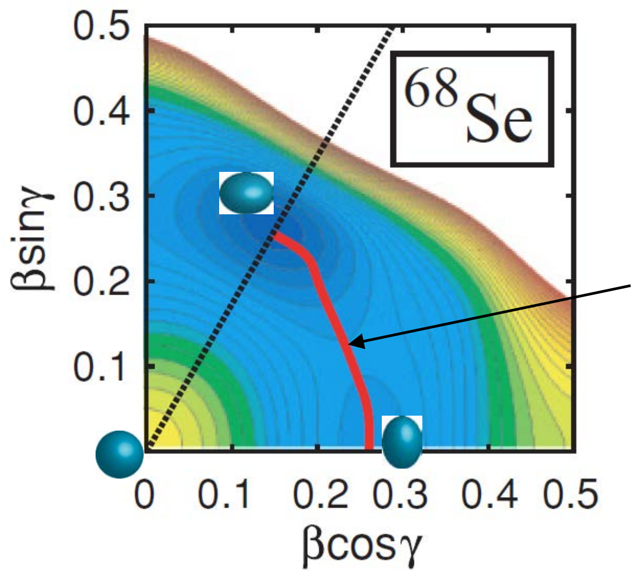
ASCC Basic Equations



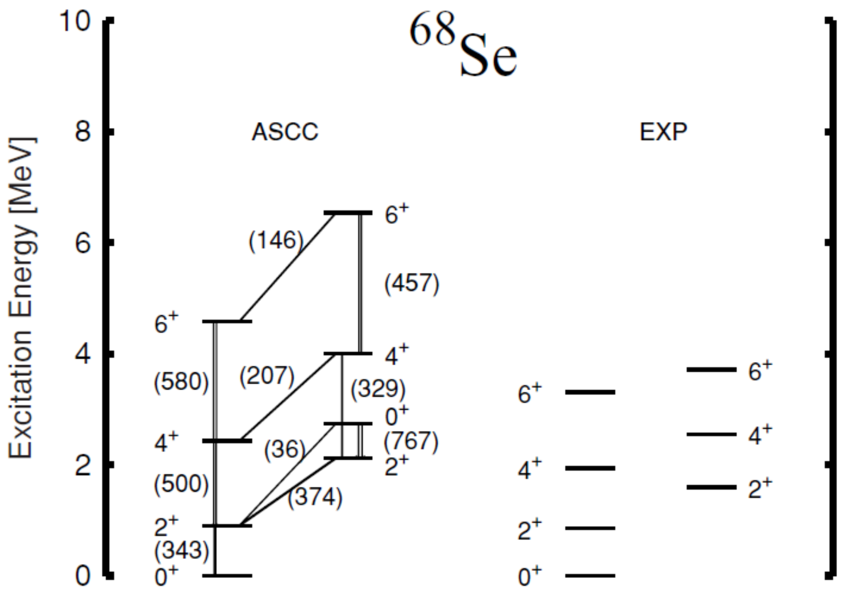
By courtesy of Hinohara-san

1D ASCC method

Hinohara et al., PTP **119**, 59 (2008); PRC 80, 014305 (2009)



“collective path”



Constrained HFB + Local QRPA method : approximate version of 2D ASCC method

⇨ microscopic determination of 5D quadrupole collective Hamiltonian

Application to large-amplitude collective dynamics in $^{68\text{-}72}$Se, $^{72\text{-}76}$Kr, $^{30\text{-}34}$Mg, $^{58\text{-}66}$Cr, etc.

N. Hinohara, K. Sato, T. Nakatsukasa, M. Matsuo, K. Matsuyanagi, PRC 82, 064313 (2010).
K. Sato and N. Hinohara, NPA 849, 53 (2011).
N. Hinohara, K. Sato, K. Yoshida, T. Nakatsukasa, M. Matsuo, and K. Matsuyanagi, PRC 84,061302 (2011).
N. Hinohara, Z. P. Li, T. Nakatsukasa, T. Niksic, D. Vretenar, PRC 85, 024323 (2012)
K. Sato, N. Hinohara, K. Yoshida, T. Nakatsukasa, M. Matsuo, and K. Matsuyanagi, PRC 86,24316 (2012).

Today's talk : extension of ASCC method including higher-order operators

State vector (w/ 1D collective coordinate and no pairing)

$$|\phi(q,p)\rangle = e^{i\hat{G}(q,p)}|\phi(q)\rangle$$

Generalized Thouless' thm

Any Slater det. can be written in the form of $e^{i\hat{G}}|\phi\rangle$ with $\hat{G}$, which is a linear combination of $a^\dagger a^\dagger$and aa terms (A-terms). $|\phi\rangle$ is a vacuum w.r.t. a. $(a|\phi(q)\rangle = 0)$

No $a^\dagger a$ term (B-term) is necessary.

Thouless,Nucl. Phys. 21 (1960) 225.
Marumori+, PTP 64 (1980) 1294

A-terms : $a^\dagger a^\dagger$ and aa terms
B-terms : $a^\dagger a$ and $aa^\dagger$ terms (or equivalently $a^\dagger a$ and constant)

Expansion $\hat{G}$ up to the 1st order of p, $\hat{G}(q,p) = p\hat{Q}(q)$ (original ver. of ASCC)

$\hat{Q}$: linear combination of A-terms

Invariance principle of Schroedinger eq. $\delta\langle\phi(q,p)|i\partial_t - \hat{H}|\phi(q,p)\rangle = 0$

$$\begin{cases} \mathcal{H} = \langle\phi(q,p)|\hat{H}|\phi(q,p)\rangle \\ \mathring{P} = i\partial_q \\ \mathring{Q} = -i\partial_p \end{cases}$$

Eq. of collective submanifold (ECS) $\delta\langle\phi(q,p)|\hat{H} - \frac{\partial\mathcal{H}}{\partial p}\mathring{P} - \frac{\partial\mathcal{H}}{\partial q}\mathring{Q}|\phi(q,p)\rangle = 0$

Adiabatic expansion in powers of p

EoM of ASCC

Matsuo, Nakatsukasa, Matsuyanagi, PTP 103(2000), 959.

Moving-frame HF equation O(1)

$$\delta\langle\phi(q)|\hat{H} - \partial_q V\hat{Q}(q)|\phi(q)\rangle = 0,$$

Moving-frame RPA equations O(p) & O(p^2)

$$\delta\langle\phi(q)|[\hat{H} - \partial_q V\hat{Q}, \hat{Q}] - \frac{1}{i}B\hat{P}|\phi(q)\rangle = 0, \qquad (\hat{P} = i\partial_q)$$

$$\delta\langle\phi(q)|[\hat{H} - \partial_q V\hat{Q}, \frac{1}{i}B\hat{P}] - BC\hat{Q} - \frac{1}{2}\partial_q V[[\hat{H} - \partial_q V\hat{Q}, \hat{Q}], \hat{Q}]|\phi(q)\rangle = 0,$$

Collective Hamiltonian $\mathcal{H} = \langle\phi(q,p)|\hat{H}|\phi(q,p)\rangle = \frac{1}{2}B(q)p^2 + V(q)$

$$V(q) = \langle\phi(q)|\hat{H}|\phi(q)\rangle$$

$$B(q) = -\langle\phi(q)|[[\hat{H}, \hat{Q}(q)], \hat{Q}(q)]|\phi(q)\rangle$$

Collective Schroedinger eq.

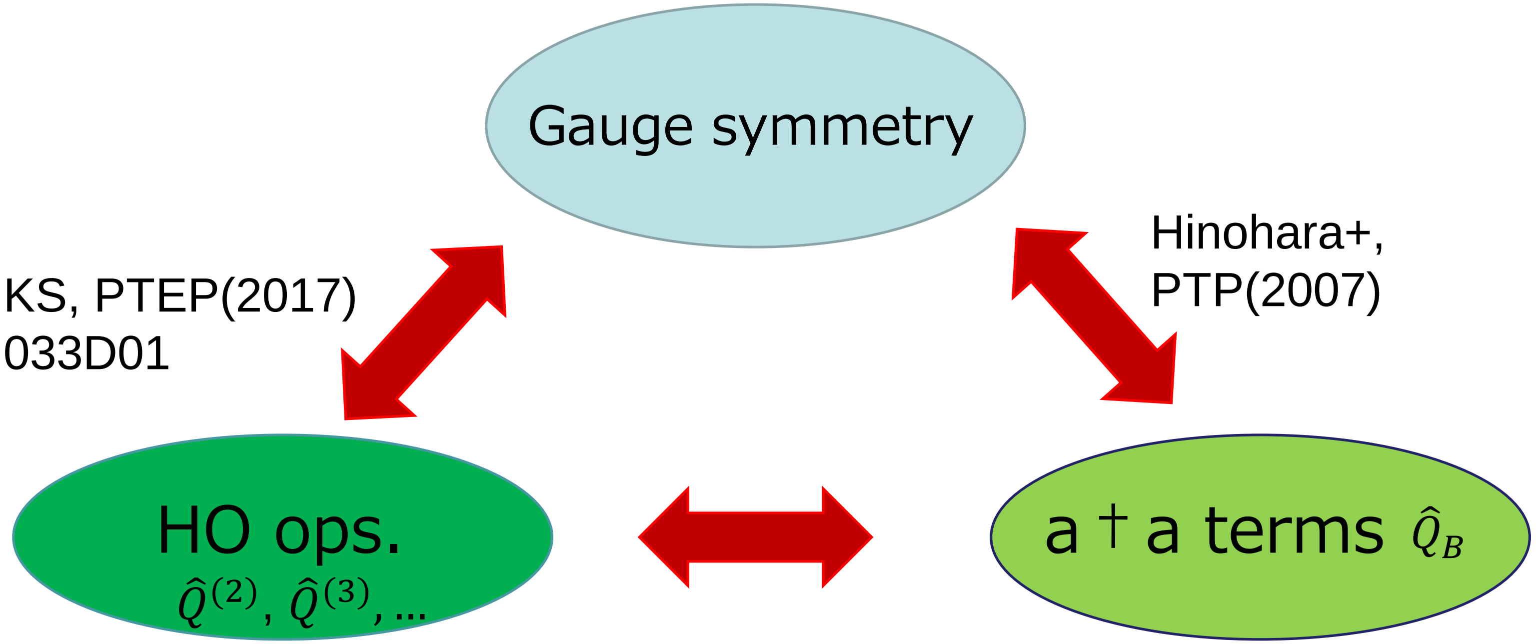
Extension including pairing correlation is NOT straightforward.

➡ One needs to introduce B-terms or HO collective operators: $\exp[ip(\hat{Q}_A + \hat{Q}_B)]|\phi(q)\rangle$

or $\exp[i(p\hat{Q}^{(1)} + \frac{1}{2}p^2\hat{Q}^{(2)} + \cdots)]|\phi(q)\rangle$

Recent findings:

KS, PTEP(2015) 123D01



$\hat{G} = p\hat{Q}^{(1)} + \frac{1}{2}p^2\hat{Q}^{(2)} \cdots$

KS, PTEP (2017) 123D03.

$\hat{Q}(q) = \hat{Q}_A(q) + \hat{Q}_B(q),$

- Before the adiabatic expansion, the gauge symmetry is kept in the EoM. To conserve the gauge symmetry, HO or a†a terms are necessary.
- Inclusion of $\hat{Q}_B$ is equivalent to that of a certain kind of higher-order collective ops. e.g. $\hat{Q}^{(2)} = i[\hat{Q}_B, \hat{Q}_A]$

Background:

Villars' ATDHF paper in 1977 , NPA 285(1977) 269.

1st - and 3rd – order ops. (No 2nd)

To satisfy the third condition, arising from the p^2 terms in (4.9), one will have to generalize the structure of $\phi(t)$, replacing $\exp(ip\hat{Q})$ by $\exp(ipQ_0+\frac{1}{3}ip^3Q_1)$. The operator $\hat{Q}_1$ will then be determined by the third condition. This extension will be presented in a separate paper [17]).

17) A. Toukan and F. Villars, to be published

Not published after all.

Baranger-Veneroni's ATDHF paper, Ann. Phys. 114 (1978) 123.

They proposed the decomposition of the density matrix as

$$\rho(t) = e^{i\chi(t)}\rho_0(t)e^{-i\chi(t)}$$

with Hermitian and time-even ρ_0 and χ.

They emphasized that χ can be written in terms of only A-terms, but included B-terms as well as A-terms in the treatment of translational motion.

The necessity of the HO terms or B-terms had been recognized already in ATDHF in 1970's.
There has been no general theory to determine them.

ASCC eqs. with HO ops. (no pairing for simplicity)

$$|\phi(q,p)\rangle = e^{i\hat{G}(q,p)}|\phi(q)\rangle \quad \text{w/} \quad \hat{G} = p\hat{Q}^{(1)} + \frac{1}{2}p^2\hat{Q}^{(2)} + \frac{1}{3!}p^3\hat{Q}^{(3)}\cdots$$

Collective operators consist of only A-terms

Moving-frame HF eq. O(1)

$$\delta\langle\phi(q)|\hat{H} - \partial_q V\hat{Q}^{(1)}|\phi(q)\rangle = 0.$$

No contribution from HO terms

Moving-frame RPA eq. of O(p)

$$\delta\langle\phi(q)|[\hat{H},\hat{Q}^{(1)}] - \frac{1}{i}B(q)\hat{P} - \underline{\frac{1}{i}\partial_q V\hat{Q}^{(2)}}|\phi(q)\rangle = 0.$$

$\hat{Q}^{(2)}$ contributes to EoM of O(p) as well as EoM of O(p^2).

Moving-frame RPA eq. of O(p^2)

$$\delta\langle\phi(q)|[\hat{H} - \partial_q V\hat{Q}^{(1)}, \frac{1}{i}B\hat{P}] - B(q)C(q)\hat{Q}^{(1)}$$

$$-\frac{1}{2}\partial_q V\left\{[[\hat{H},\hat{Q}^{(1)}],\hat{Q}^{(1)}] + \underline{[\hat{H},\frac{1}{i}\hat{Q}^{(2)}] + \partial_q V\left(\hat{Q}^{(3)} + \frac{1}{2}[\hat{Q}^{(1)},\frac{1}{i}\hat{Q}^{(2)}]\right.}\right)\Bigg\}|\phi(q)\rangle = 0.$$

Contributions from HO operators are not "higher-order" contribution.

“1 + 1 >> 2” ?

(inverse) inertial mass

$$B(q) = -\langle\phi(q|[[\hat{H},\hat{Q}^{(1)}],\hat{Q}^{(1)}]|\phi(q)\rangle + \underline{\langle\phi(q|[\hat{H},i\hat{Q}^{(2)}]|\phi(q)\rangle}$$

$\hat{Q}^{(2)}$ does contribute to the inertial mass.

Although it is of the same order as the first term,
the second term has been neglected conventionally (or maybe even not recognized).

Can we really ignore the second-order operator ? ⇨ Let's include the 2nd-order op. $\hat{Q}^{(2)}$ (but neglect $\hat{Q}^{(3)}$).

When $\hat{Q}^{(2)}$ is included, we need one more equation to determine it.
How can we determine $\hat{Q}^{(2)}$?

ASCC EoM consist of 3 equations derived from 4 equations

Eq. of collective submanifold (ECS)

$$\delta\langle\phi(q,p)|\hat{H} - \frac{\partial\mathcal{H}}{\partial p}\mathring{P} - \frac{\partial\mathcal{H}}{\partial q}\mathring{Q}|\phi(q,p)\rangle = 0$$

⇨ Expand in powers of p

①0th-order eq.

→ moving-frame HF eq.

②1st-order eq.

→ moving-frame RPA eq. of O(p)

④2nd-order eq. + ③derivative of 0th –order eq.

→ moving-frame RPA eq. of $O(p^2)$

Basic equations (w/o pairing)

Eq. of collective submanifold (ECS)

$$\delta\langle\phi(q,p)|\hat{H}-\frac{\partial\mathcal{H}}{\partial p}\mathring{P}-\frac{\partial\mathcal{H}}{\partial q}\mathring{Q}|\phi(q,p)\rangle=0$$

①0th-order ECS [moving-frame HF eq.]　O(1)

$$\delta\langle\phi(q)|\hat{H}-\partial_q V\hat{Q}^{(1)}|\phi(q)\rangle=0.$$

②1st-order ECS [moving-frame RPA eq. of O(p)]　O(p)

$$\delta\langle\phi(q)|[\hat{H},\hat{Q}^{(1)}]-\frac{1}{i}B(q)\hat{P}-\frac{1}{i}\partial_q V\hat{Q}^{(2)}|\phi(q)\rangle=0.$$

③ q-derivative of the 0th-order ECS　Eq. of "O(q)"

$$\delta\langle\phi(q)|[\hat{H}-\partial_q V\hat{Q}^{(1)},\frac{1}{i}B(q)\hat{P}]-B(q)C(q)\hat{Q}^{(1)}-\partial_q VB(q)\underline{D_q\hat{Q}^{(1)}}|\phi(q)\rangle=0$$

may be approximated by finite difference

④2nd-order ECS　O(p²)　[with $\hat{Q}^{(3)}$ omitted]

$$\delta\langle\phi(q)|\frac{1}{2}[[\hat{H},\hat{Q}^{(1)}],\hat{Q}^{(1)}]-B(q)\underline{D_q\hat{Q}^{(1)}}-\frac{i}{2}[\hat{H},\hat{Q}^{(2)}]-\frac{i}{4}\partial_q V[\hat{Q}^{(1)},\hat{Q}^{(2)}]|\phi(q)\rangle=0,$$

- The moving-frame RPA of O(p²) eq. is derived by eliminating $D_q\hat{Q}^{(1)}$ from ③ with use of ④.
- We adopt ④ as an independent eq. as well as ③.

①, ②, ③+④　ASCC eqs. w/o $Q^{(2)}$ (original)

↓

①, ②, ③, ④　ASCC eqs. w/ $Q^{(2)}$ (new)

Illustration w/ (2-level) Lipkin model

Lipkin, Nucl. Phys. 62(1965) 188.

Holzwarth, Nucl. Phys. A 207(1973) 545.

$$\hat{H} = \frac{1}{2}\epsilon \sum_{p>0} \left[a_p^\dagger a_p - (1 - a_{-p}^\dagger a_{-p}) \right] + \frac{1}{2} V \sum_{p,p'>0} \left(a_p^\dagger a_{p'}^\dagger a_{-p'}^\dagger a_{-p}^\dagger + \text{h.c.} \right)$$

$$= \epsilon \hat{K}_0 + \frac{1}{2} V \left(\hat{K}_+ \hat{K}_+ + \hat{K}_- \hat{K}_- \right)$$

quasispin:

$$\hat{K}_0 = \frac{1}{2} \sum_{p>0} \left[a_p^\dagger a_p - a_{-p} a_{-p}^\dagger \right] \quad \hat{K}_+ = \sum_{p>0} a_p^\dagger a_{-p}^\dagger, \; \hat{K}_- = \hat{K}_+^\dagger$$

$$[\hat{K}_+, \hat{K}_-] = 2\hat{K}_0, \;\; [\hat{K}_0, \hat{K}_\pm] = \pm \hat{K}_\pm$$

particle and hole ops. ↔ nucleon ops.

$$a_p = c_p, \qquad a_p^\dagger = c_p\dagger,$$

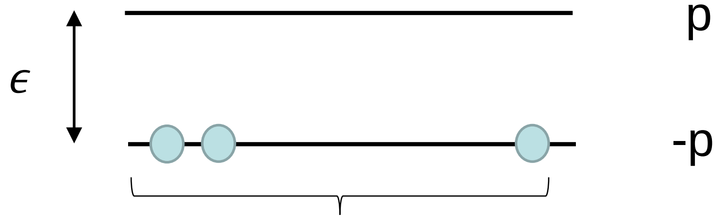
$$a_{-p} = c_{-p}^\dagger \qquad a_{-p}^\dagger = c_{-p}$$

2-level Lipkin model

N-fold degeneracy & N particles

Non-interacting case

$$a_{\pm p}|0\rangle = 0$$ g. s. w/ V=0



Lower level fully
occupied by N particles

Interacting case

"deformed" op.:

$$\begin{pmatrix} \alpha_p^\dagger \\ \alpha_{-p} \end{pmatrix} = \begin{pmatrix} \cos\frac{\phi}{2} & -\sin\frac{\phi}{2} \\ \sin\frac{\phi}{2} & \cos\frac{\phi}{2} \end{pmatrix} \begin{pmatrix} a_p^\dagger \\ a_{-p} \end{pmatrix}$$

"deformed" state:

$$|\phi\rangle = \mathcal{N} \exp\left[\left(\tan\frac{\phi}{2}\right)\hat{K}_+\right] |0\rangle$$

Vacuum for V=0

Vacuum w. r. t. deformed op.

$$\alpha_{\pm p}|\phi\rangle = 0$$

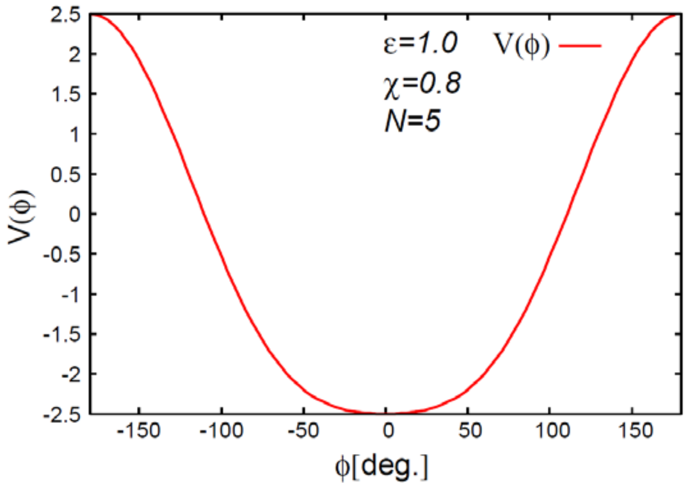
Collective potential V(ϕ)

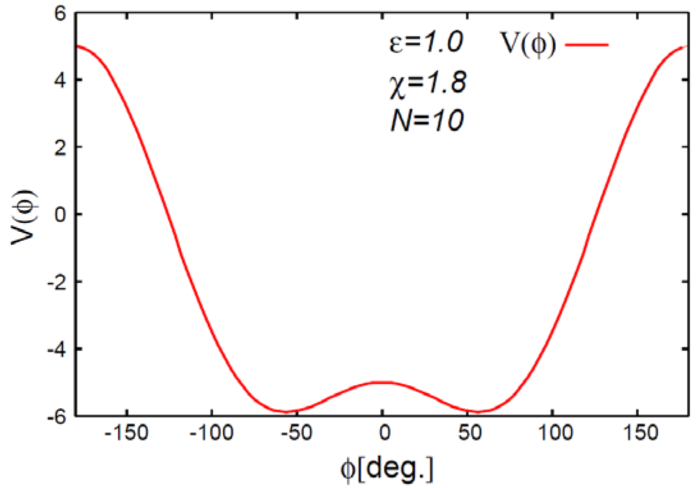
$$V(\phi) = \langle\phi|\hat{H}|\phi\rangle$$

$$= -\frac{N}{2}\epsilon(\cos\phi + \frac{1}{2}\chi\sin^2\phi)$$

with $\chi = (1-N)V/\epsilon$

χ<1 "spherical" → "deformed" χ >1





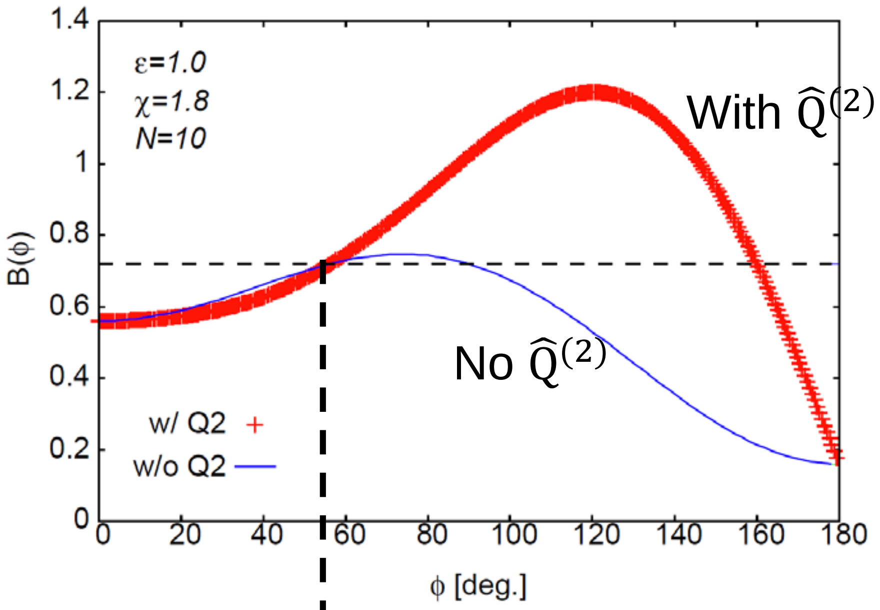
"Phase transition" as a function of χ

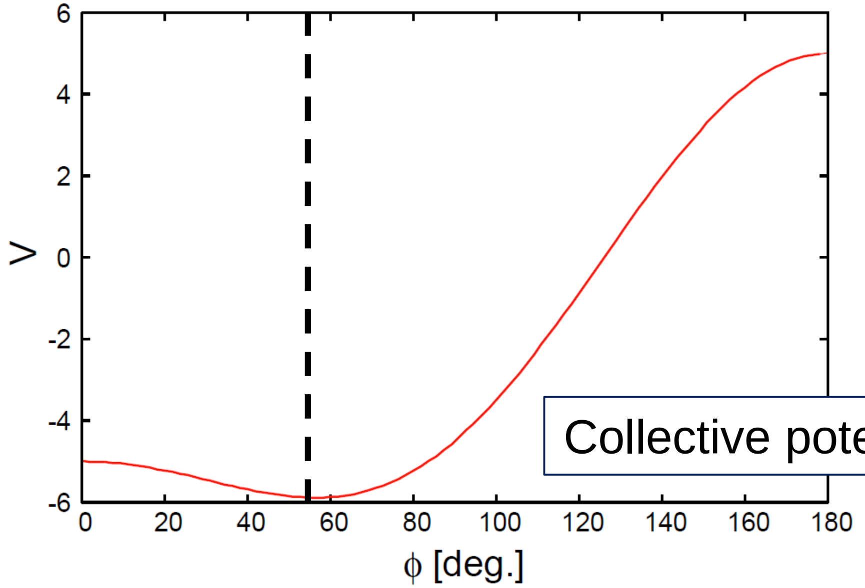
HF eq.: $\frac{\partial V}{\partial \phi} = \frac{N}{2}\epsilon\sin\phi\,(1-\chi\cos\phi) = 0.$

Inverse mass $B(\phi) = 1/M(\phi)$

$$\mathcal{H} = \frac{1}{2}M(\phi)\dot{\phi}^2 + V(\phi) \qquad \hat{Q}^{(1)}(q) = Q^{(1)}(q)(\hat{J}_+(q) + \hat{J}_-(q))$$

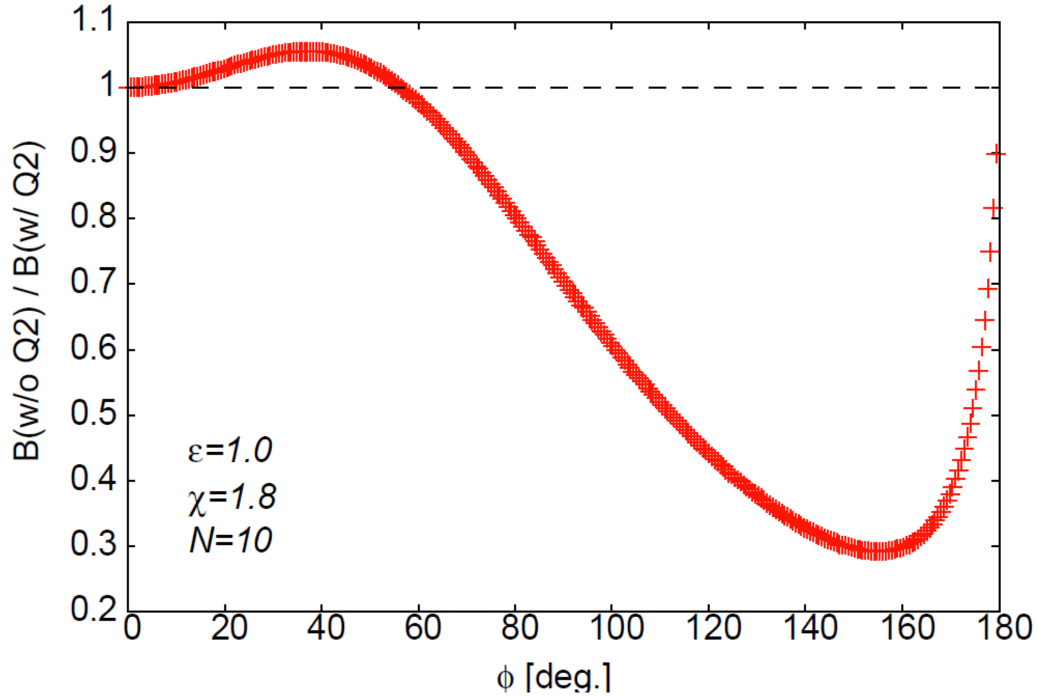
$$M(\phi) = N^2\left(Q^{(1)}\right)^2$$





Collective potential $V(\phi)$

Ratio of the two: $\dfrac{M(\phi)\text{ w/ }Q^{(2)}}{M(\phi)\text{ w/o }Q^{(2)}}$



Difference can be by the factor of 3 approximately

Results calculated with $\chi = 1.8, \varepsilon = 1.0, N = 10$

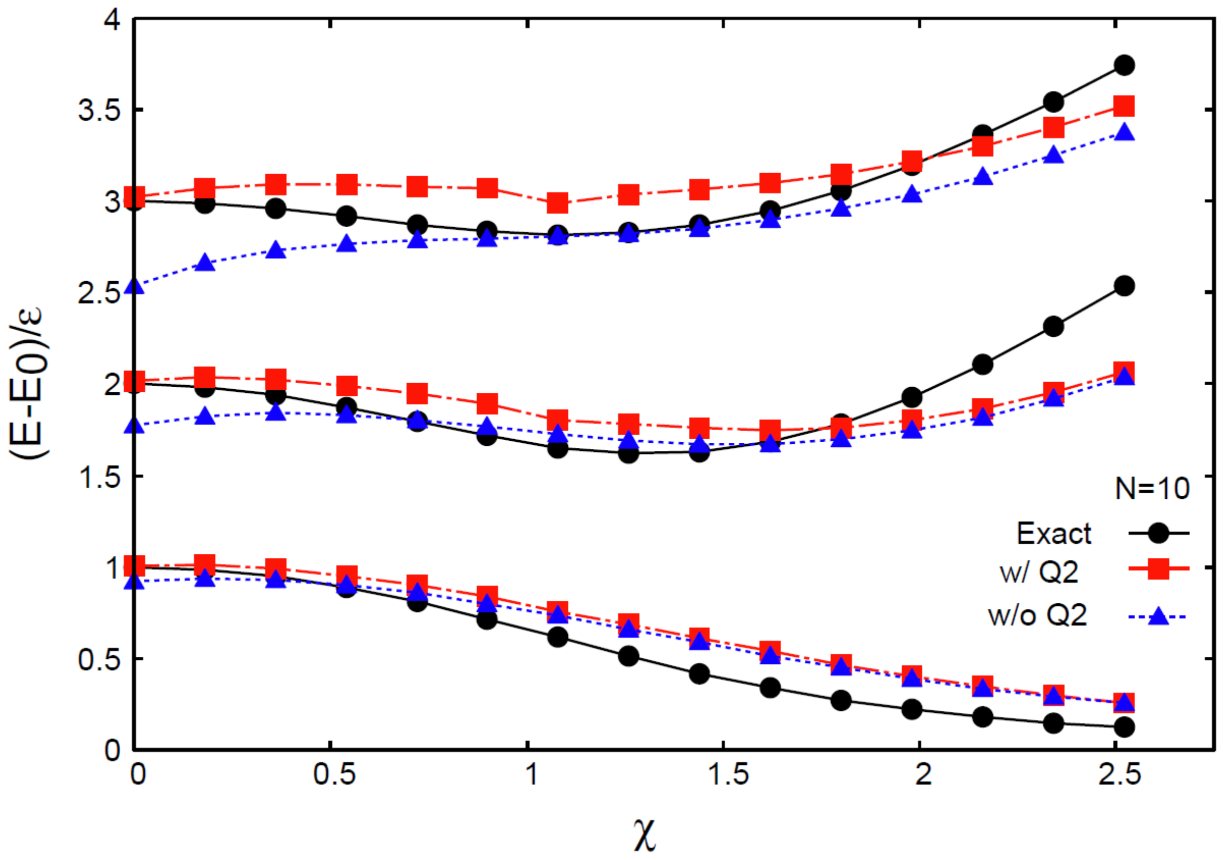
	Exact	No Q(2)	With Q(2)		No Q(2)	With Q(2)
	Excitation energies				Deviation from exact solution	
	exact	mfRPA w/o $Q^{(2)}$	mfRPA w/ $Q^{(2)}$	$\delta E/E \times 100$	$\Delta E/\epsilon$ (w/o $Q^{(2)}$)	$\Delta E/\epsilon$ (w/ $Q^{(2)}$)
E_0	0	0	0		0	0
E_1	0.27204	0.4482	0.46639	4.1	0.17616	0.19435
E_2	1.784	1.6947	1.7599	3.8	-0.0893	-0.0241
E_3	3.058	2.9592	3.1423	6.2	-0.0988	0.0843
E_4	4.6112	4.3496	4.7177	8.4	-0.2616	0.1065
E_5	6.2235	5.7586	6.3816	12	-0.4649	0.1581
E_6	7.8358	7.1242	7.9945	12	-0.7116	0.1587
E_7	9.389	8.3993	9.703	16	-0.9897	0.314
E_8	10.663	9.4164	10.455	11	-1.2466	-0.208
E_9	12.175	10.606	12.972	22	-1.569	0.797
E_{10}	12.447	10.803	12.989	20	-1.644	0.542

Q(2) improves the agreement with the exact solution！Good agreement for higher excited states.

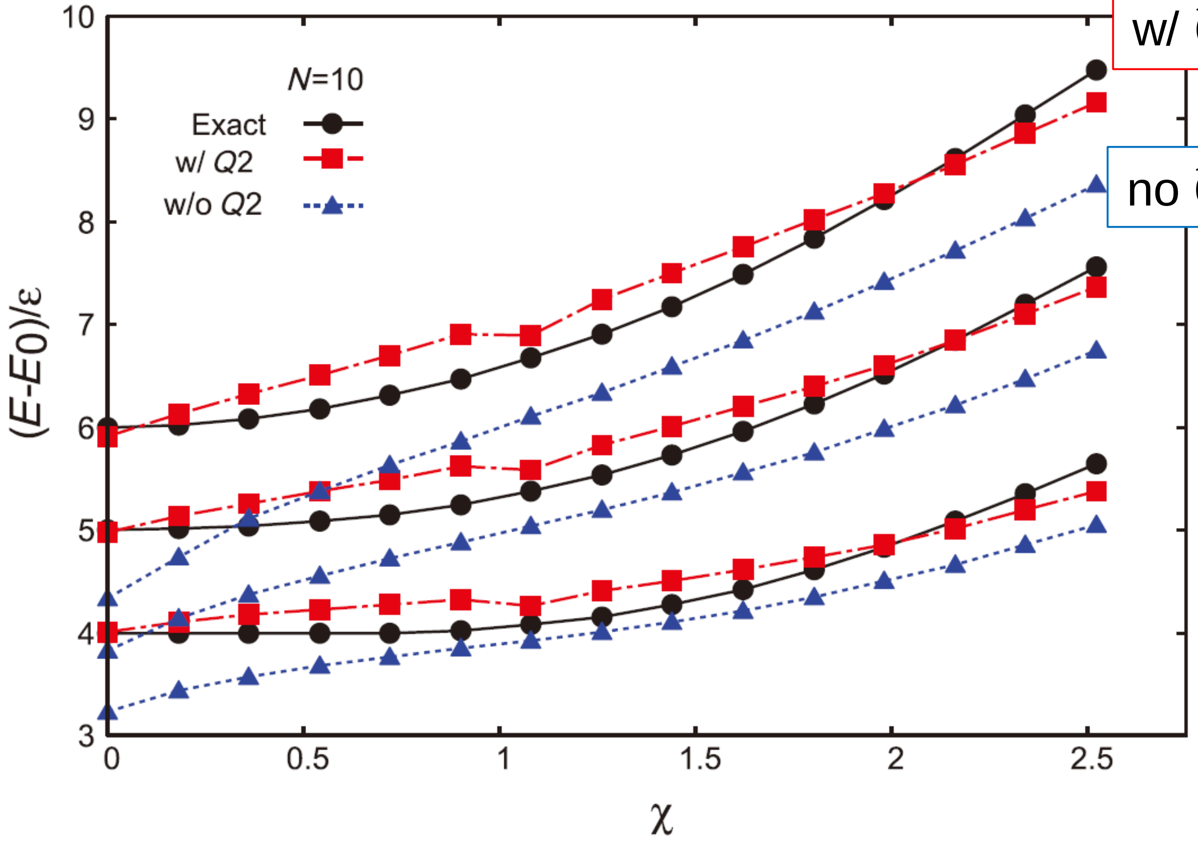
Comparison of excitation energies $(N = 10)$

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

the 1st, 2nd, 3rd excited states



the 4th, 5th, 6th excited states



w/ $\hat{Q}^{(2)}$

no $\hat{Q}^{(2)}$

- Both reproduce the exact solution rather well for first few excited states.
- Without $\hat{Q}^{(2)}$, the excitation energies are systematically underestimated for higher excited states.
- With $\hat{Q}^{(2)}$, the exact solution is well reproduced even for higher excited states.

Summary :

- The higher-order operators contribute to the inertial mass and the equations of motion.
- We have proposed a new set of basic equations to determine the second-order collective–coordinate operator $\hat{Q}^{(2)}$ and applied it to the Lipkin model.
- For a first few excited states, the difference between the calculations with and without $\hat{Q}^{(2)}$ is not significant.
- With $\hat{Q}^{(2)}$ included, the agreement with the exact solution is good even for highly-excited states.
- The set of basic equations proposed here can treat both of the cases with and without pairing on an equal footing.

- The gauge is fixed in the new set of basic equations. (No numerical instability expected)

⇨ Application to systems w/ pairing would be interesting.