
# The emergence of multi-phonon giant resonances within a fully quantum TDDFT framework

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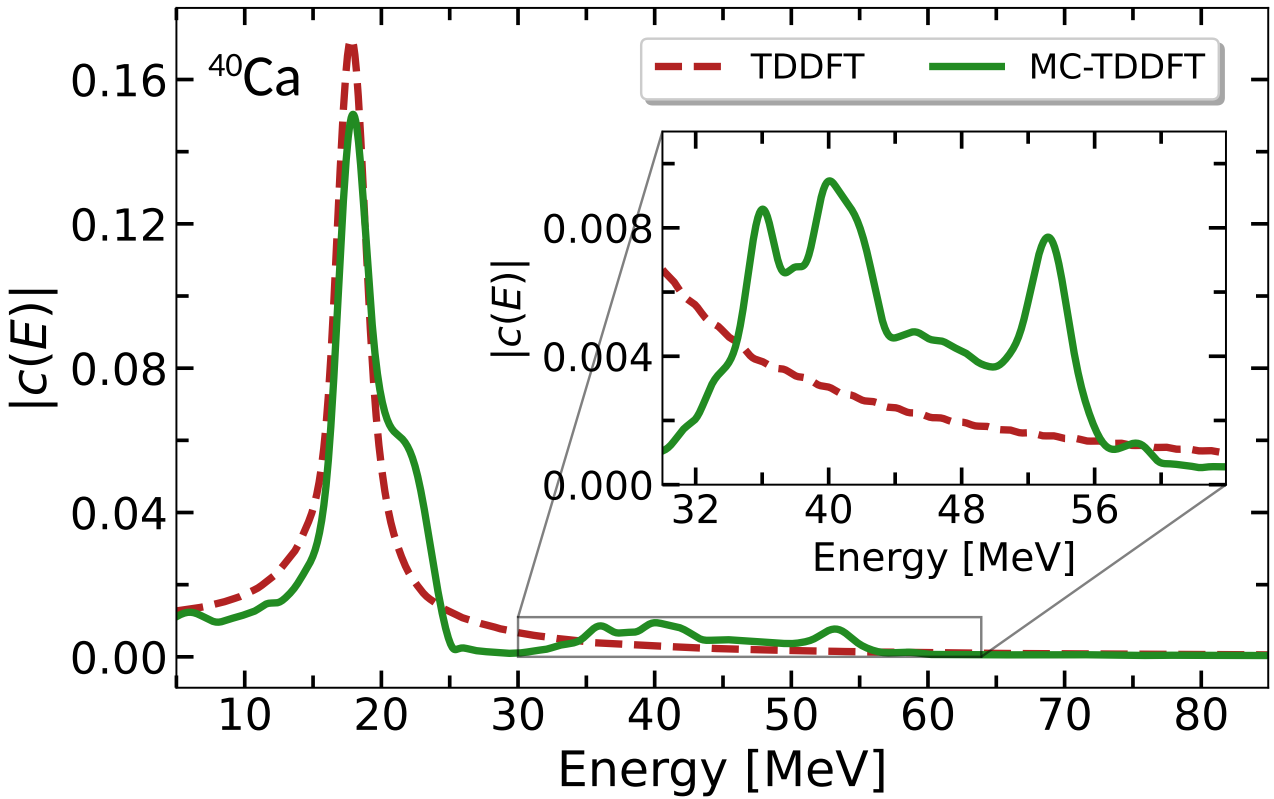
# Peaks at nearly 2x and 3x the energy of the main ISGQR peak!



# Outline

1. A tale of two models
2. The MC-TDDFT model
3. ISGQR multi-phonons in $^{40}Ca$

# A tale of two models

# A tale of two models

- Today, there are two popular types of microscopic models of nuclear dynamics

**Time-dependent density functional theory**

$$|\Psi(t)\rangle = |\Phi_q(t)\rangle$$

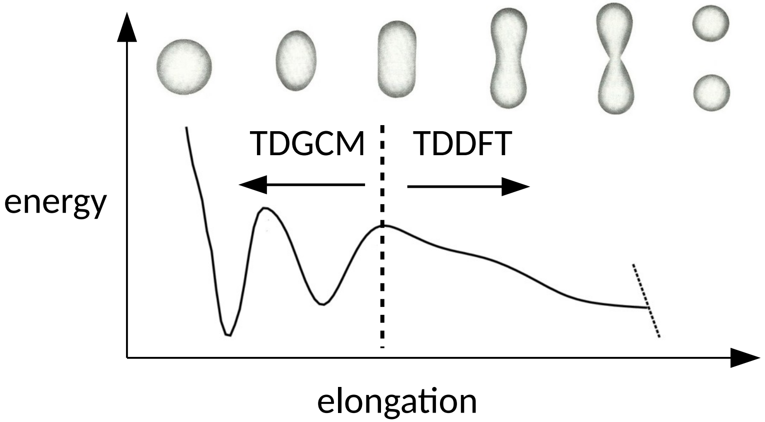
Dissipation, but no fluctuations
(Quasi-classical)

**Time-dependent generator coordinate method**

$$|\Psi(t)\rangle = \int dq f_q(t) \, |\Phi_q\rangle$$

Fluctuations, but no dissipation
(Adiabatic)

**Illustration: 1D PES in fission**




The idea is to **leverage the advantages od both types of models**.

- Pioneering work done by Reinhard and collaborators in the early 1980s
- Recently, a renewed interest: Regnier and Lacroix (2019), Hasegawa *et al.* (2020)
- However, so far, there were no realistic applications in atomic nuclei

# The MC-TDDFT model

# The MC-TDDFT model

- Multiconfigurational TDDFT:

$$|\Psi(t)\rangle = \int dq f_q(t) \, |\Phi_q(t)\rangle$$

$f_q(t)$ = mixing functions, determined by the variational principle

$|\Phi_q(t)\rangle$ = basis states, e.g. HF or HFB

**Time dependence is in both the mixing functions and the basis states!**

- Equations of motion for mixing functions and basis states

$$i\hbar\dot{g} = \left(\mathcal{H}^c - \mathcal{D}^c + i\hbar\dot{\mathcal{N}}^{1/2}\mathcal{N}^{-1/2}\right) g$$

$$i\hbar\dot{\rho}_q(t) = \Big[h[\rho_q(t)], \rho_q(t)\Big]$$

| | |
|---|---|
| Hamiltonian kernel | $\mathcal{H}_{qq'}(t) = \left\langle \Phi_q(t) \middle| \hat{H} \middle| \Phi_{q'}(t) \right\rangle$ |
| norm kernel | $\mathcal{N}_{qq'}(t) = \langle \Phi_q(t) \, | \Phi_{q'}(t) \rangle$ |
| time derivative kernel | $\mathcal{D}_{qq'}(t) = \langle \Phi_q(t) \, | i\hbar\partial_t | \, \Phi_{q'}(t) \rangle$ |
| collective kernels | $\mathcal{O}^c(t) = \mathcal{N}^{-1/2}(t)\mathcal{O}(t)\mathcal{N}^{-1/2}(t)$ |
| collective wave functions | $g(t) = \mathcal{N}^{1/2}(t) f(t)$ |

# The MC-TDDFT model

- Numerical resolution for $g_q(t)$ gives an access to various observables

$$\left\langle \Psi(t) \left| \hat{O} \right| \Psi(t) \right\rangle = \iint dq dq' g_q^*(t) \mathcal{O}^c_{qq'}(t) g_{q'}(t)$$

Some properties of the model:

- Fully quantum (accounts for fluctuations in the collective space)
- Diabatic (dissipation effects, much smaller bases may be needed)
- Can describe for both the small- and large-amplitude collective motion
- Does not include superfluidity, for now
- Implemented in a new code (modern C++, finite elements method)

Based on this model, we performed the first MC-TDDFT calculations in nuclei.

*P. M., David Regnier, and Denis Lacroix, arXiv:2304.07380 [nucl-th] (April 2023)*
*“Quantum fluctuations induce collective multi-phonons in finite Fermi liquids”*

# ISGQR multi-phonons in $^{40}Ca$

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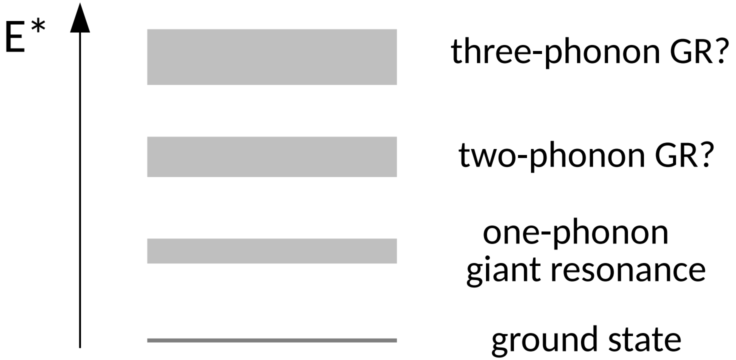
## Multi-phonons in atomic nuclei

- Multi-phonons: higher quanta of the main GR excitation?




**Scheme of a hypothetical multi-phonon spectrum**

Do collective multi-phonon excitations exist in nuclei?

Are they harmonic?

**There are many decades of excellent research on the topic!**

<u>Experiment</u>:

- 2$^{nd}$ phonon observed in multiple nuclei
- 3$^{nd}$ phonon possibly observed in two cases
  - Schmidt *et al.*, IVGDR in $^{136}$Xe (1993) (?)
  - Fallot *et al.*, ISGQR in $^{40}$Ca (2006)

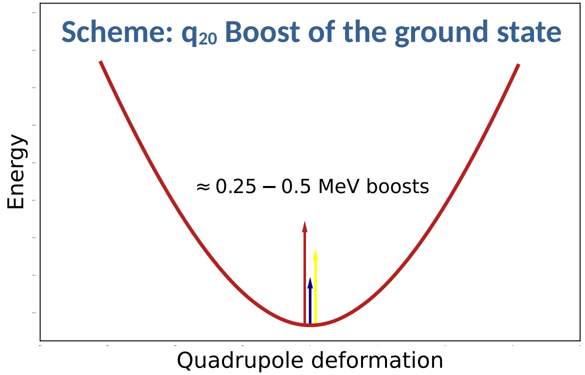
<u>Theory</u>:

- In principle, a (re-)quantized theory is needed
- Many models on the market, usually an *ad hoc* introduction of phonon degrees of freedom

# ISGQR multi-phonons in $^{40}Ca$
## Calculation parameters

- Some calculation parameters:
  - L = 24 fm box, regular mesh of 14 cells, FE basis of 3rd order polynomials
  - SLy4d Skyrme EDF (well-suited for dynamical studies)
  - Basis states correspond to the HF ground state with different $q_{20}$ boosts

- We consider a simple case of quantum configuration mixing




**At *t* = *0***

TDDFT $$|\Psi(0)\rangle = \exp(i\lambda\hat{Q})\,|\Phi_{\mathrm{GS}}\rangle$$

MC-TDDFT $$|\Psi(0)\rangle = \exp(i\lambda\hat{Q})\Big(f_1(0)\,|\Phi_{\mathrm{GS}}\rangle + f_2(0)\,|\Phi_2(0)\rangle + f_3(0)\,|\Phi_3(0)\rangle\Big)$$

**At later *t***

TDDFT $$|\Psi(t)\rangle = |\Phi_1(t)\rangle$$

MC-TDDFT $$|\Psi(t)\rangle = f_1(t)\,|\Phi_1(t)\rangle + f_2(t)\,|\Phi_2(t)\rangle + f_3(t)\,|\Phi_3(t)\rangle$$

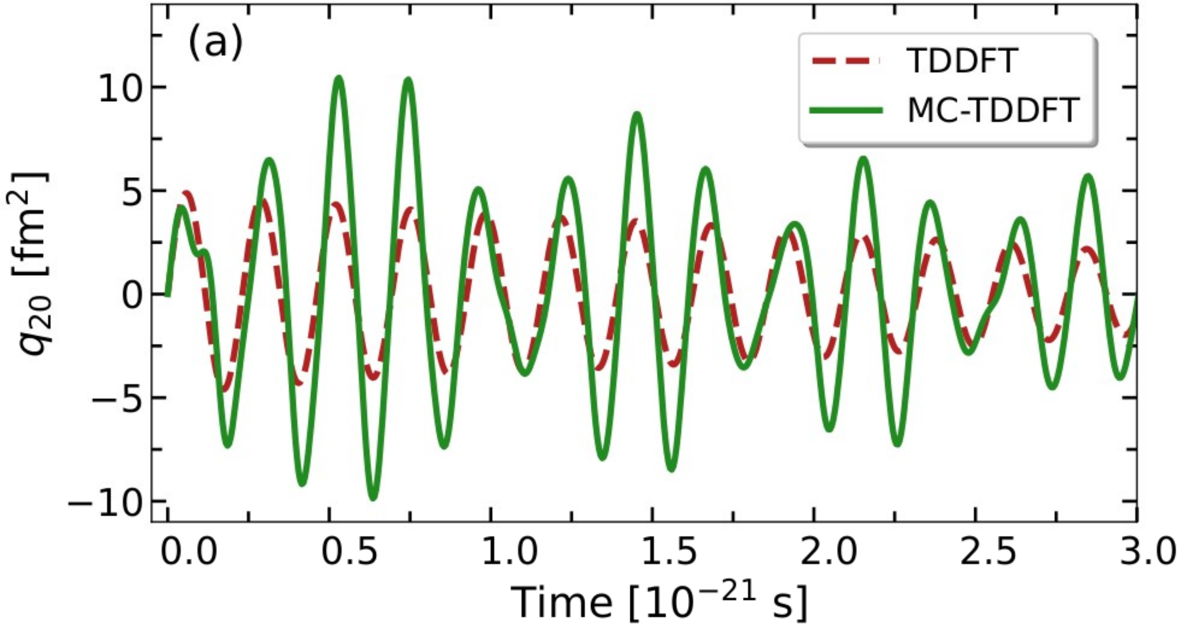
$$f_1(0) = 1 \qquad f_2(0) = f_3(0) = 0$$

We can compare predictions of the **quasi-classical TDDFT** and the **quantum MC-TDDFT**.

# ISGQR multi-phonons in $^{40}Ca$

## Nuclear response to a quadrupole perturbation

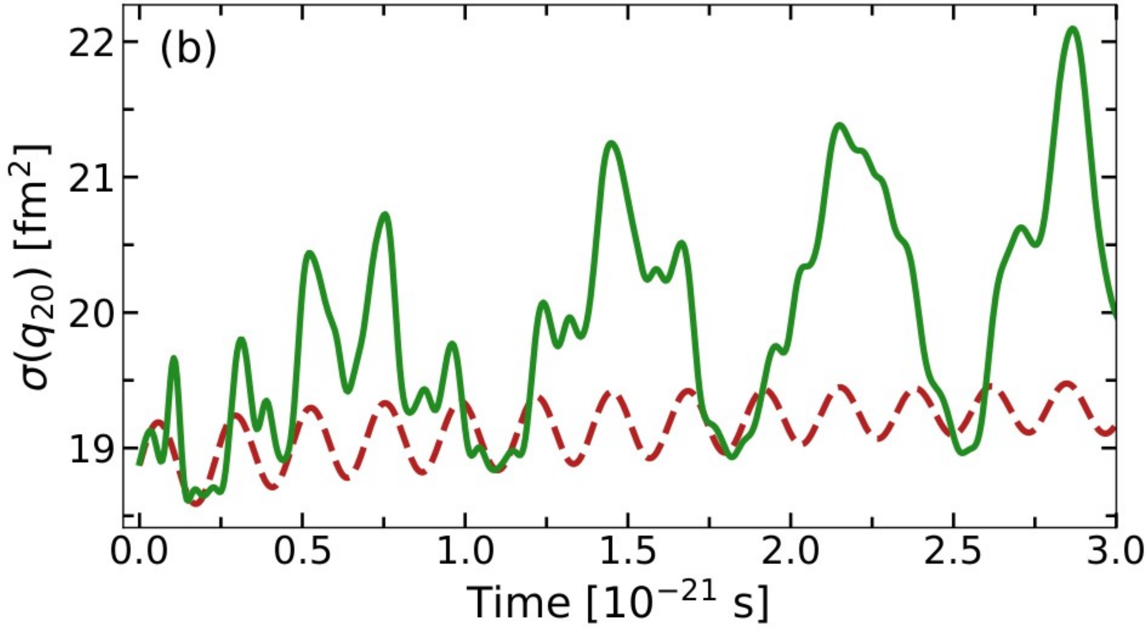
- Quadrupole response for MC-TDDFT is **more complex** and exhibits **multiple frequencies**



# ISGQR multi-phonons in $^{40}Ca$

## Nuclear response to a quadrupole perturbation

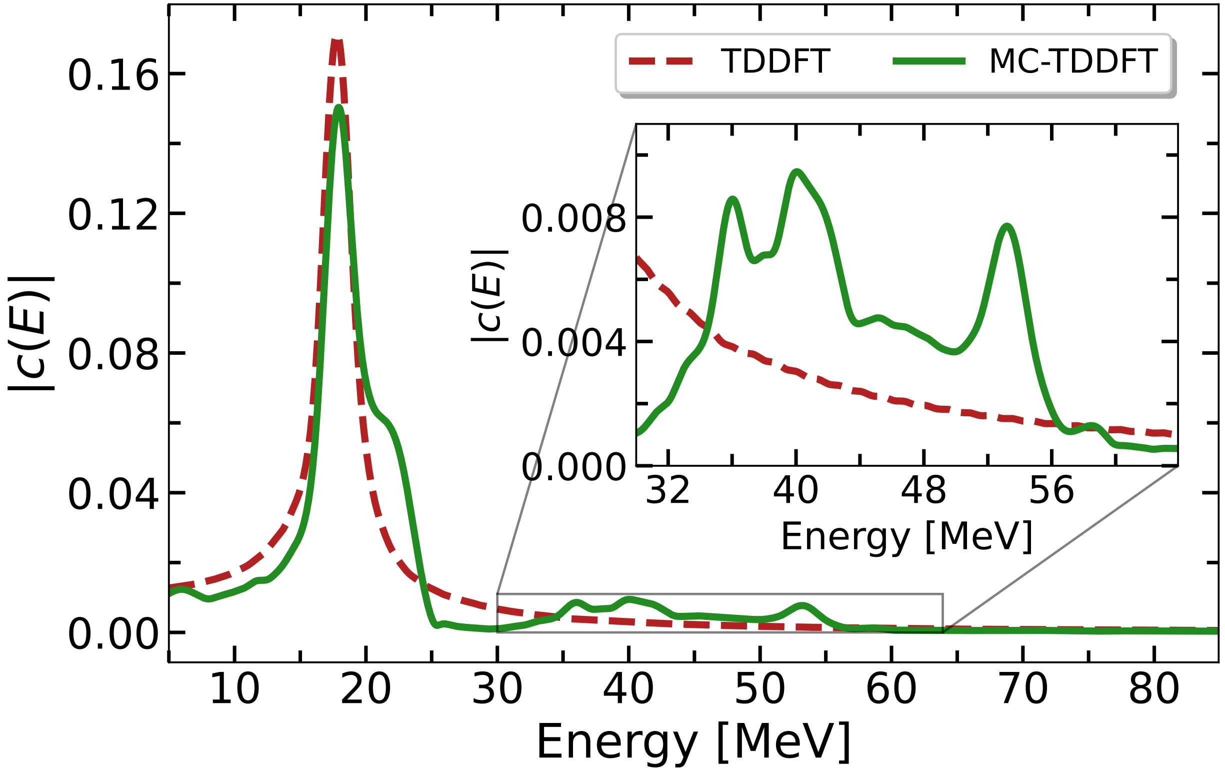
- Quadrupole response for MC-TDDFT is **more complex** and exhibits **multiple frequencies**
- Quadrupole fluctuations are **larger** and also exhibit multiple frequencies
- Frequency (energy) spectrum can be extracted through Fourier analysis



# ISGQR multi-phonons in $^{40}Ca$

## Energy spectrum

- TDDFT yields a **single peak** (other trajectories are equivalent)
- MC-TDDFT yields **multiple peaks**
  - The 1st peak is split (but we do not aim to describe all the fine details!)
  - The 2nd and 3rd peak appear at 2x and 3x the energy and reflect this splitting
  - There is no 4th peak



# ISGQR multi-phonons in $^{40}Ca$

## Robustness of results

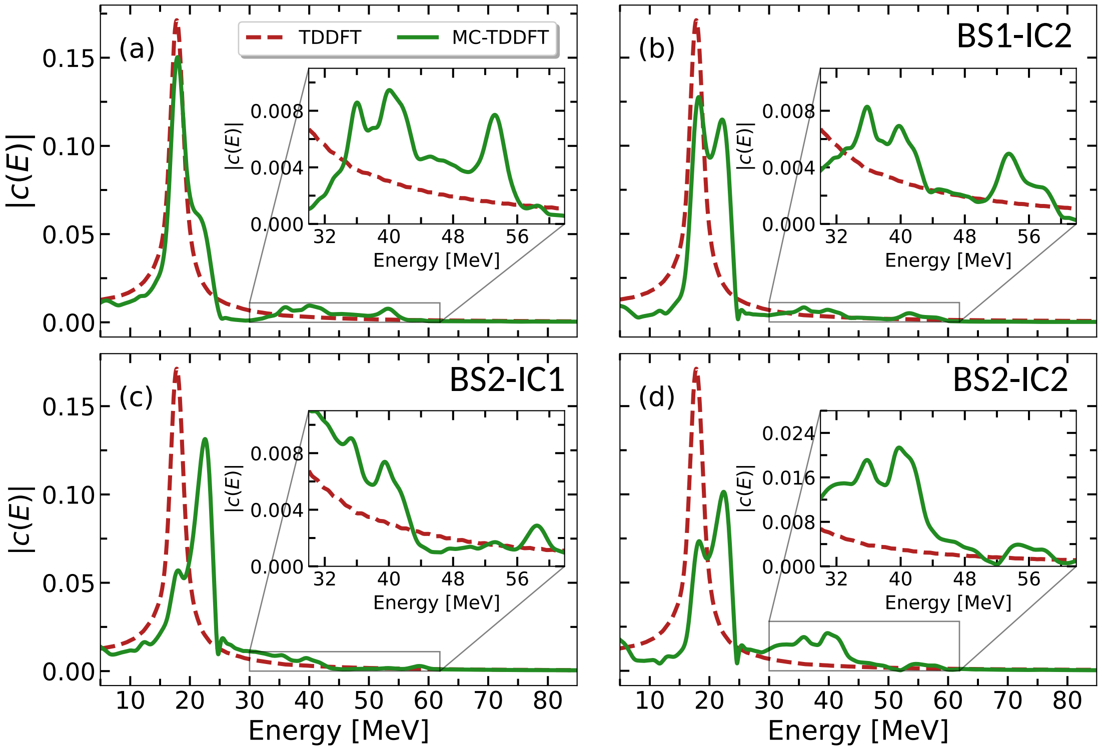
- To test robustness, we considered two sets of basis states and two sets of initial conditions

**Basis States 1** – Different boost magnitudes

**Basis States 2** – The same boost, different points along the trajectory

**Init. Conditions 1** – $f_1(0) = 1$, $f_2(0) = f_3(0) = 0$

**Init. Conditions 2** – Diagonalization of the initial collective Hamiltonian

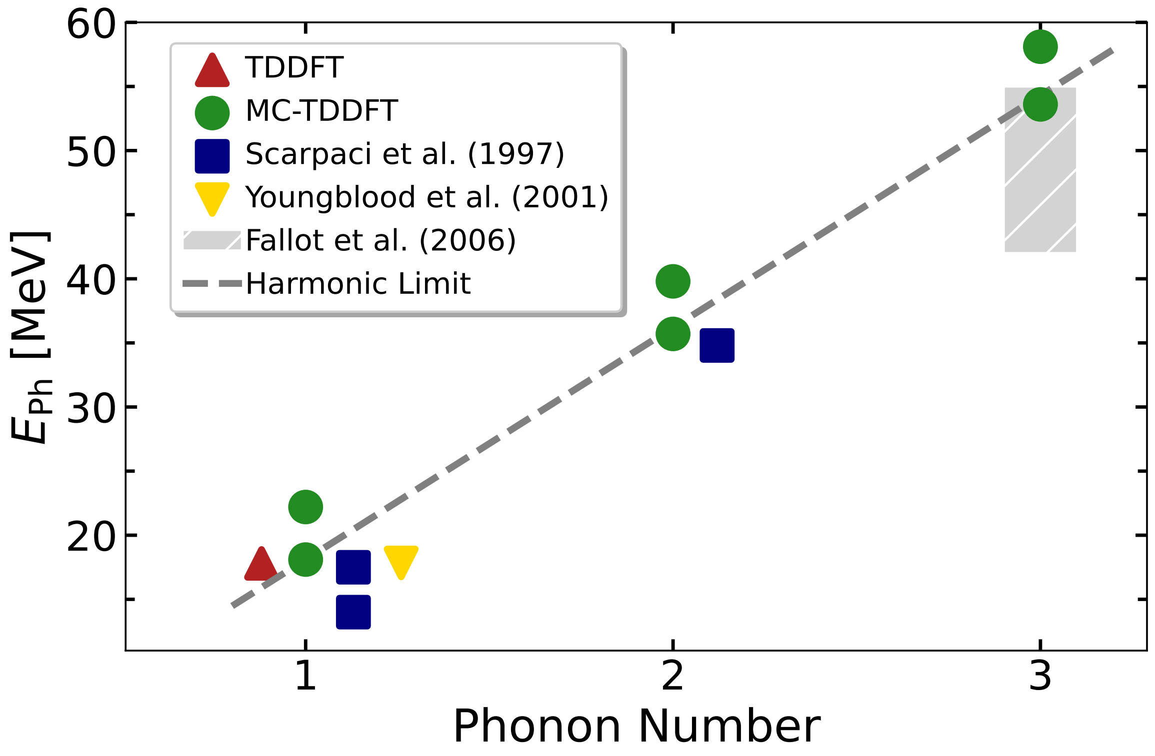



The appearance of peaks and their energies are **robust** with respect to this choice (but amplitudes vary).

# ISGQR multi-phonons in $^{40}Ca$

## Comparison with the experiment

Excitation energies are in **excellent agreement** with experiment and **nearly harmonic** (~2%).




**Excitations of the main peak:**

$E_{1ph}$ = 18.1 (0.2) MeV

$E_{2ph}$ = 35.7 (0.4) MeV

$E_{3ph}$ = 53.6 (0.7) MeV

(not full theoretical uncertainties!)

# Takeaways

1) The first MC-TDDFT model in atomic nuclei is up and running.

2) A simple re-quantized model predicts collective, nearly-harmonic ISGQR multi-phonons in $^{40}Ca$.

3) Further extensions (pairing) are a very promising avenue for modeling more complex dynamical phenomena.

**Thank you!**