# Emergence of collective motion

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# Outline

Binding and excitation energies with JISP16

Electromagnetic observables with JISP16

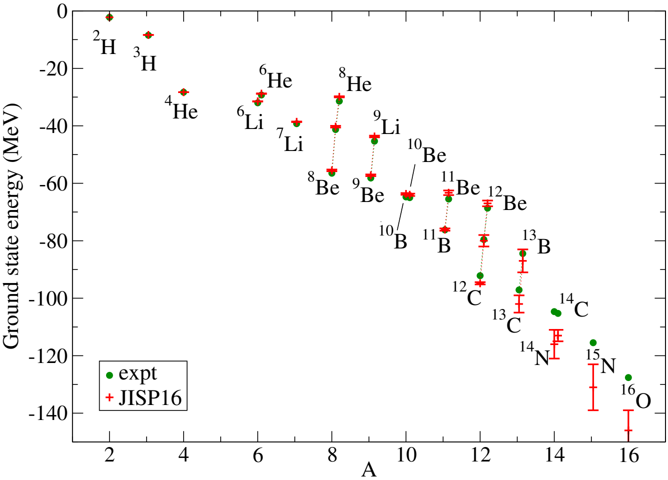
Emergence of rotational bands

Detailed example: $^9$Be

Intrinsic rotational band paramereters

# Ground state energies of *p*-shell nuclei with JISP16

Maris and Vary, IJMPE22, 1330016 (2013)



# Extrapolating to complete basis

Challenge: achieve numerical convergence for No-Core CI calculations using a finite amount of CPU time on current HPC systems

- Perform a series of calculations with increasing $N_{\max}$ truncation
- Extrapolate to infinite model space $\longrightarrow$ exact results
  - Empirical: binding energy exponential in $N_{\max}$

$$E^{N}_{\text{binding}} = E^{\infty}_{\text{binding}} + a_1 \exp(-a_2 N_{\max})$$

  - use 3 or 4 consecutive $N_{\max}$ values to determine $E^{\infty}_{\text{binding}}$
  - use $\hbar\omega$ and $N_{\max}$ dependence to estimate numerical error bars

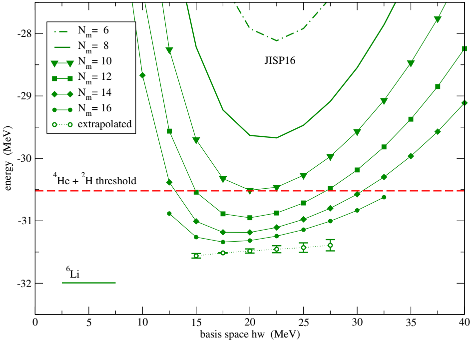
Maris, Shirokov, Vary, PRC79, 014308 (2009)

- Recent studies of IR and UV behavior based on S.P. asymptotics: exponentials in $\sqrt{\hbar\omega/N}$ and $\sqrt{\hbar\omega N}$

Coon *et al*, PRC86, 054002 (2012);
Furnstahl, Hagen, Papenbrock, PRC86, 031301(R) (2012);
More, Ekstrom, Furnstahl, Hagen, Papenbrock, PRC87, 044326 (2013);
Wendt, Forssén, Papenbrock and Sääf, PRC91, 061301 (2015);
More, PhD thesis OSU, arXiv:1608.01385 [nucl-th];

# Extrapolating to complete basis – in practice

- Perform a series of calculations with increasing $N_{\max}$ truncation



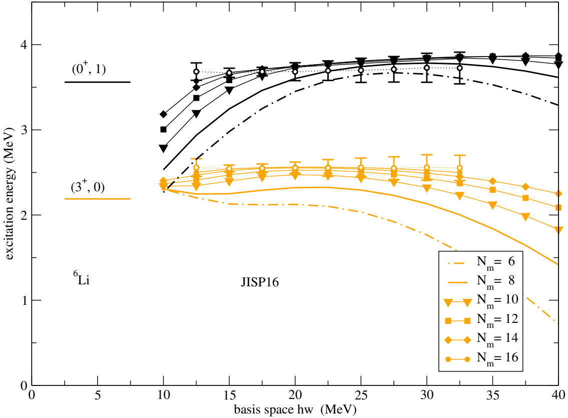

- H.O. basis up to $N_{\max} = 16$ and exponential extrapilation $E_b = -31.49(3)$ MeV

Cockrell, Maris, Vary, PRC86, 034325 (2012)

- Hyperspherical harmonics up to $K_{\max} = 14$: $E_b = -31.46(5)$ MeV

Vaintraub, Barnea, Gazit, PRC79, 065501 (2009)

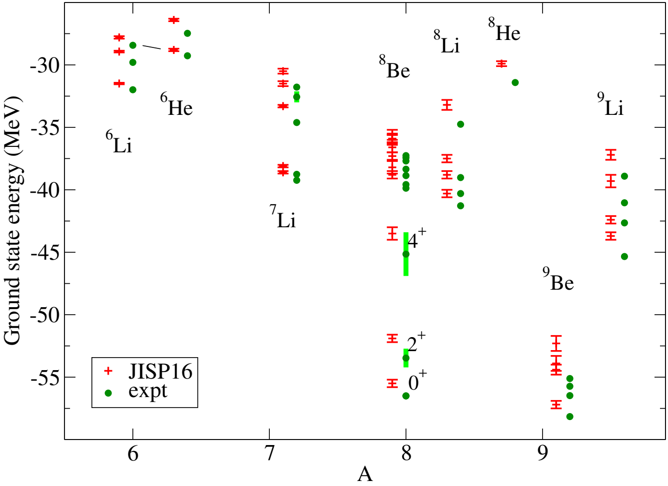
# Spectrum of $^6$Li




- Excitation energies narrow states reasonably well converged
- No need for extrapolations

# Energies of excited states of $A = 6$ to $A = 9$ nuclei

Maris and Vary, IJMPE22, 1330016 (2013)



# Local one-body density

- One-body density in single-particle coordinates

$$\rho(\vec{r}) \;=\; \int |\Psi(\vec{r}_1, \vec{r}_2, \ldots, \vec{r}_A)|^2 \, d^3 r_2 \ldots d^3 r_A$$

- Lab-frame density $\rho^\omega(\vec{r})$ includes Center-of-Mass motion

$$\rho^\omega(\vec{r}) \;=\; \int \rho_{\text{rel}}(\vec{r} - \vec{R}) \, \rho^\omega_{\text{CM}}(\vec{R}) \, d^3 \vec{R}.$$

  - depends on basis $\hbar\omega$, even in complete (infinitely large) basis
- Deconvolution of relative density and Center-of-Mass motion

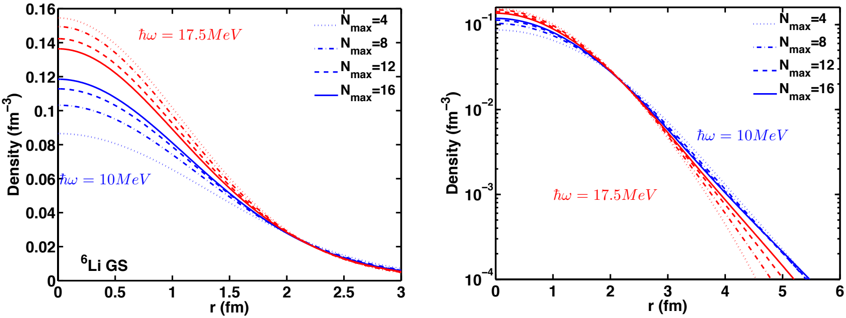
$$\rho_{\text{rel}}(\vec{r}) \;=\; F^{-1}\left[\frac{F[\rho^\omega(\vec{r})]}{F[\rho^\omega_{\text{CM}}(\vec{r})]}\right]$$

- Multipole expansion (used to facilitate deconvolution)

$$\rho(\vec{r}) = \sum_{K=0}^{2J} \frac{\langle JMK0|JM\rangle}{\sqrt{2J+1}} \, Y^0_K(\theta) \, \rho^{(K)}(r)$$

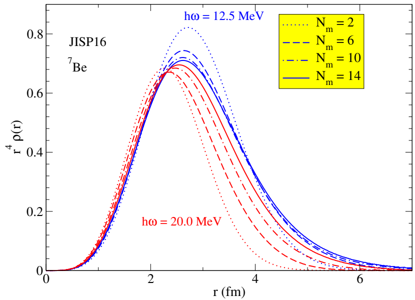
# Density of $^6$Li

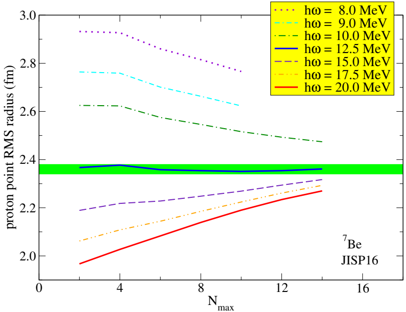
Cockrell, Maris, Vary, PRC86, 034325 (2012)




- Slow convergence of asymptotic tail of wavefunction in particular for larger $\hbar\omega$ values
- Hence, slow convergence of RMS radii, quadrupole moments, etc.

# Radius of $^7$Be




- Calculation one-body observables $\langle i|\mathcal{O}|j\rangle \sim \int \mathcal{O}(r)\, r^2\, \rho_{ij}(r)\, dr$
- RMS radius: $\mathcal{O}(r) = r^2$
- Slow convergence of RMS radius due to slow build up of asymptotic tail
- Ground state RMS radius in agreement with data

# Multipole operators

Electric quadrupole ($E2$) operator

$$\mathbf{Q}_2 = \sum_{i=1}^{A} e_i r_i^2 Y_{2u}(\mathbf{r}_i) \quad = \quad e_p \mathbf{Q}_p + e_n \mathbf{Q}_n$$

$$e_p = e \qquad e_n = 0$$

$$\mathbf{Q}_p \sim \sum_{i=1}^{Z} r_{p,i}^2 Y_{2u}(\mathbf{r}_{p,i}) \qquad \mathbf{Q}_n \sim \sum_{i=1}^{N} r_{n,i}^2 Y_{2u}(\mathbf{r}_{n,i})$$

*Proton & neutron tensors*

Magnetic dipole ($M1$) operator

$$\mathbf{M}_1 = \sqrt{\frac{3}{4\pi}} \mu_N \sum_{i=1}^{A} (g_\ell^{(i)} \boldsymbol{\ell}_i + g_s^{(i)} s_i)$$

$$g_{\ell,p} = 1 \qquad g_{\ell,n} = 0$$

$$g_{s,p} \approx 5.585 \qquad g_{s,n} \approx -3.826$$

$$= g_{\ell,p}\mathbf{D}_{\ell,p} + g_{\ell,n}\mathbf{D}_{\ell,n} + g_{s,p}\mathbf{D}_{s,p} + g_{s,n}\mathbf{D}_{s,n},$$

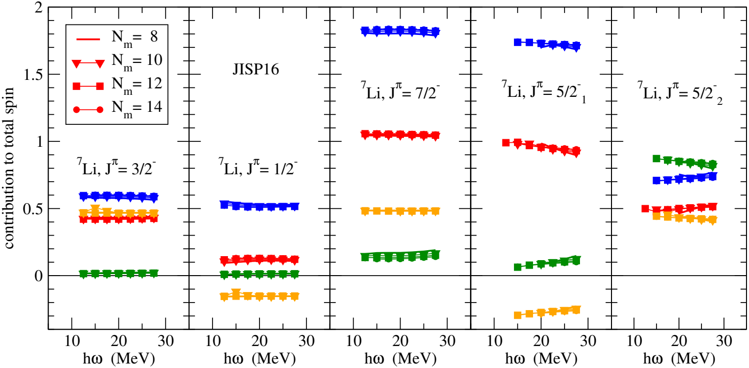
$$\mathbf{D}_{\ell,p} \sim \sum_{i=1}^{Z} \boldsymbol{\ell}_{p,i} \quad \mathbf{D}_{\ell,n} \sim \sum_{i=1}^{N} \boldsymbol{\ell}_{n,i} \quad \mathbf{D}_{s,p} \sim \sum_{i=1}^{Z} s_{p,i} \quad \mathbf{D}_{s,n} \sim \sum_{i=1}^{N} s_{n,i}$$

*Dipole terms*

# Dipole terms of $^7$Li

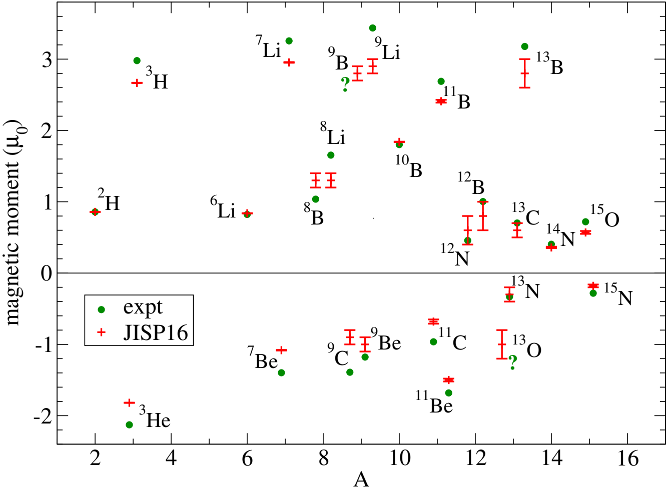
Maris, Vary, IJMPE22, 1330016 (2013)

$$J = \frac{1}{J+1}\left(\langle \vec{J}\cdot\vec{L}_p\rangle + \langle \vec{J}\cdot\vec{L}_n\rangle + \langle \vec{J}\cdot\vec{S}_p\rangle + \langle \vec{J}\cdot\vec{S}_n\rangle\right)$$




- Converged with $N_{max}$, persistent weak $\hbar\omega$ dependence $\frac{5}{2}^-$ states
- Two $\frac{5}{2}^-$ states have very different structure

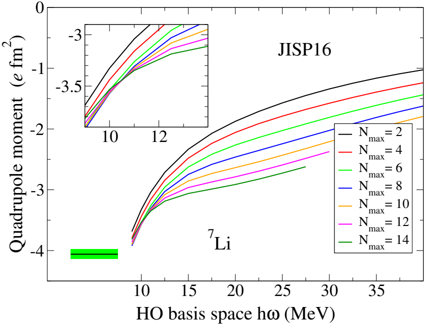
# Magnetic moments of *p*-shell nuclei with JISP16

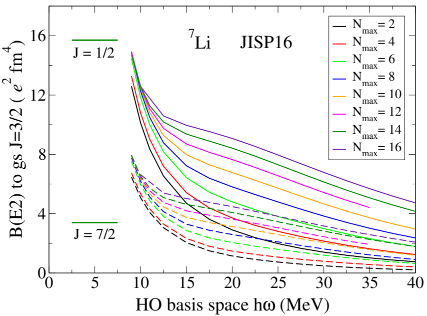



- Magnetic moments reasonably well converged
- Deviations from experiment: missing meson exchange currents

# Quadrupole moment and E2 transition strengths 7Li

Cockrell, Maris, Vary, PRC86 034325 (2012)

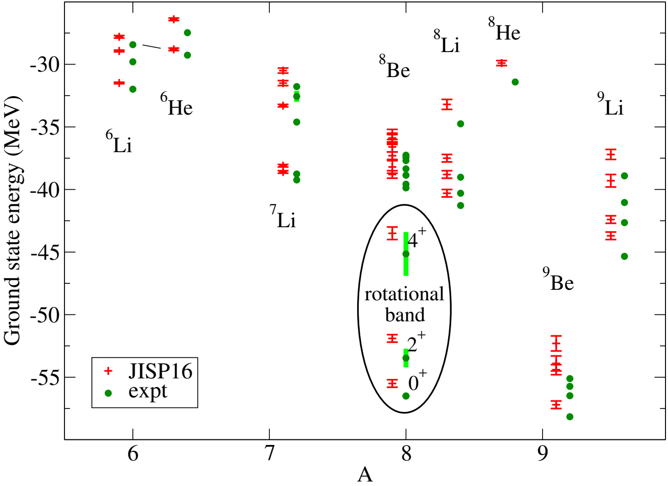



- E2 observables not converged,
  due to gaussian fall-off of HO wavefunction
- Nevertheless, qualitative agreement of $\mathcal{Q}$ and B(E2) with data

# Spectrum of $A = 6$ to 9 nuclei with JISP16

Maris and Vary, IJMPE22, 1330016 (2013)




- Rotational band?

# Rotational model predictions

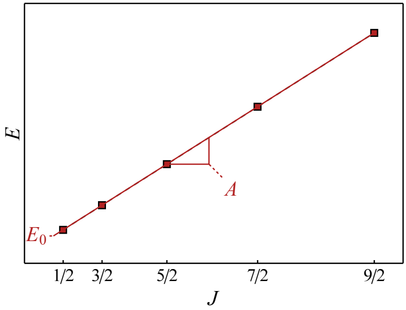
Intrinsic state $|\phi_K\rangle$ & rotation in Euler angles $\vartheta$ $(J = K, K+1, \ldots)$

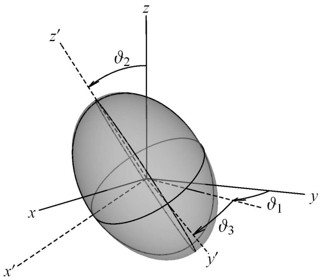
$$|\psi_{JKM}\rangle \propto \int d\vartheta \Big[ \mathscr{D}^J_{MK}(\vartheta)|\phi_K;\vartheta\rangle + (-)^{J+K}\mathscr{D}^J_{M-K}(\vartheta)|\phi_{\bar{K}};\vartheta\rangle \Big]$$

Rotational energy

$$E(J) = E_0 + A[J(J+1) + \underbrace{a(-)^{J+1/2}(J+\tfrac{1}{2})}_{\text{Coriolis } (K=1/2)}] \qquad A \equiv \frac{\hbar^2}{2\mathcal{J}}$$

Rotational relations on electromagnetic transitions $(E2, M1, \ldots)$



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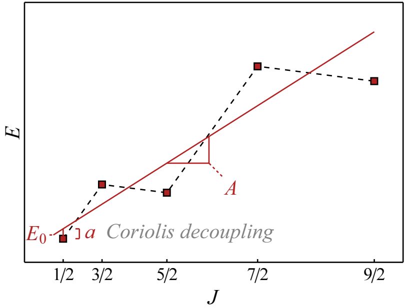
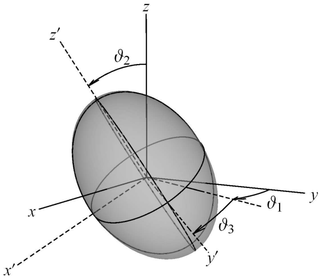
Rotational relations on electromagnetic transitions ($E2$, $M1$, ...)



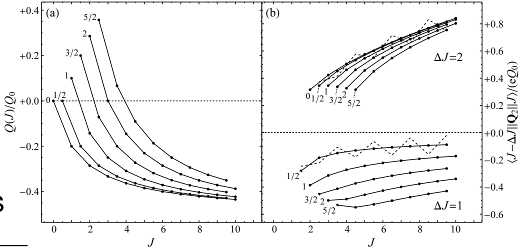



# Rotational band: Quadrupole matrix elements

$$\langle \psi_{J_f K} || E_2 || \psi_{J_i K} \rangle = \frac{(2J_i+1)^{1/2}}{1+\delta_{K0}} \Big( (J_i, K, 2, 0 | J_f, K) \, \langle \phi_K || E_{2,0} || \phi_K \rangle + (-)^{J_i+K} (J_i, -K, 2, 2K | J_f, K) \, \langle \phi_K || E_{2,2K} || \phi_{\bar{K}} \rangle \Big)$$

- Quadrupole moments

$$\mathcal{Q}(J) = \frac{3K^2 - J(J+1)}{(J+1)(2J+3)} \, \mathcal{Q}_0$$




- Transition matrix elements

$$\langle \psi_{J_f K} || E_2 || \psi_{J_i K} \rangle = \sqrt{\frac{5}{16\pi}} \sqrt{2J_i+1} \, (J_i K 2 0 | J_f K) \, \mathcal{Q}_0$$

- Consider both proton and neutron quadrupole tensors

# Rotational band: Dipole matrix elements

- Magnetic moments

$$\mu(J) = a_0\, J + a_1 \frac{K}{J+1} + a_2\, \delta_{K,\frac{1}{2}} \frac{(-1)^{J-\frac{1}{2}}}{2\sqrt{2}} \frac{2J+1}{J+1}$$

- Magnetic transition matrix elements

$$\langle \psi_{J-1,K} || M_1 || \psi_{J,K} \rangle = -\sqrt{\frac{3}{4\pi}} \sqrt{\frac{J^2-K^2}{J}} \left( a_1 + a_2\, \delta_{K,\frac{1}{2}} \frac{(-1)^{J-\frac{1}{2}}}{\sqrt{2}} \right)$$

- Define dipole terms $D_{l,p}$, $D_{l,n}$, $D_{s,p}$, and $D_{s,n}$ for both the magnetic moments and for the $M_1$ transitions

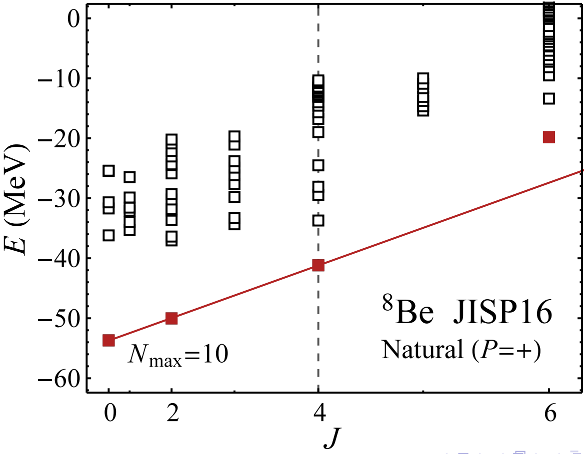
$$M_1 = g_{l,p}\, D_{l,p} + g_{l,n}\, D_{l,n} + g_{s,p}\, D_{s,p} + g_{s,n}\, D_{s,n}$$

with $g_{l,p} = 1$, $g_{l,n} = 0$, $g_{s,p} = 5.586$, and $g_{s,n} = -3.826$

# $^8$Be ground state rotational band

*Shell model:* Valence space angular momentum $J \leq 4$

*Cluster model:* Molecular rotation of $\alpha + \alpha$ dimer



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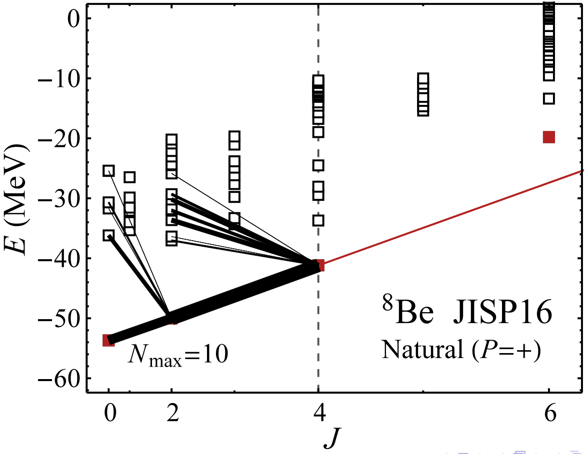

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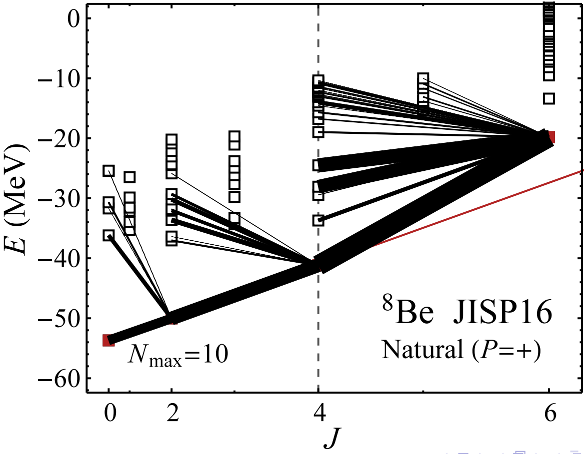
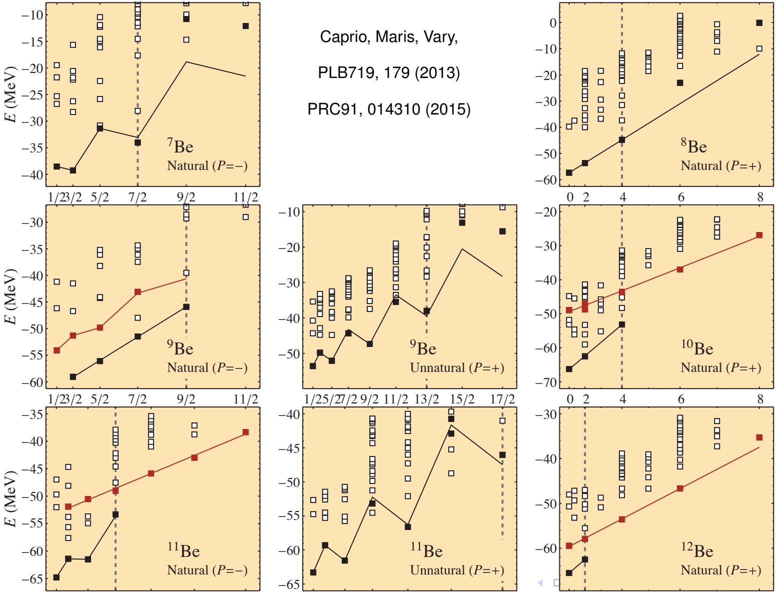


# Candidate Rotational bands in Be isotopes

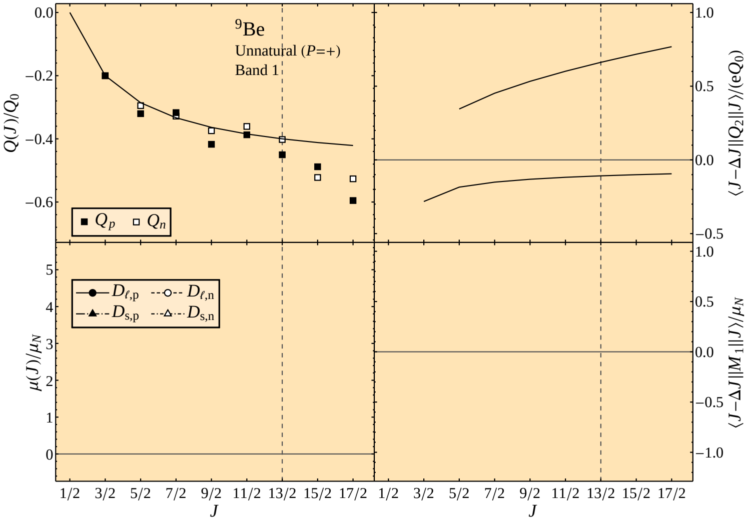
Caprio, Maris, Vary,

PLB719, 179 (2013)

PRC91, 014310 (2015)

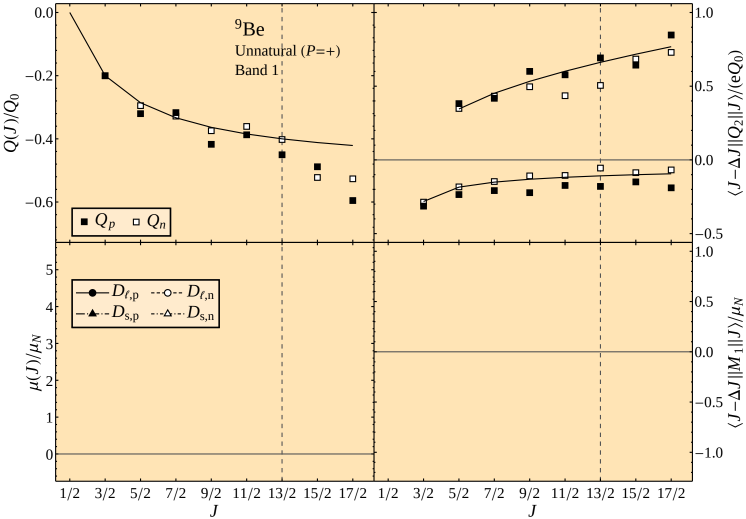


# E2 moments

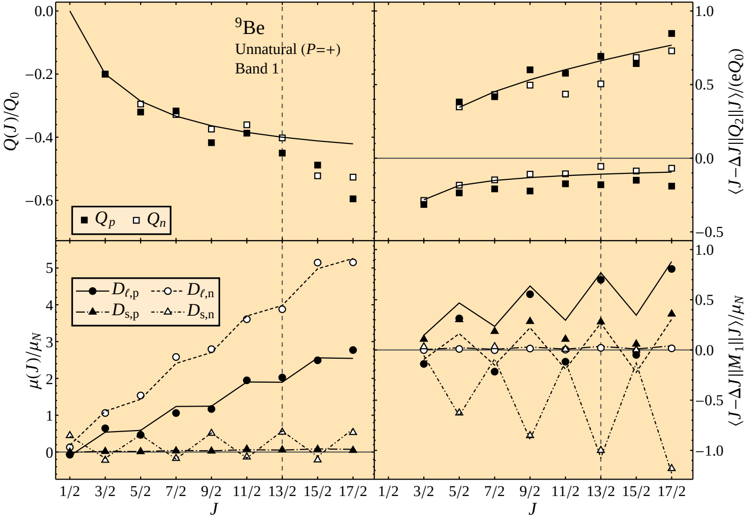


$^9$Be
Unnatural ($P$=+)
Band 1
$Q_p$ $Q_n$
$Q(J)/Q_0$
$\langle J-\Delta J||Q_2||J\rangle/(eQ_0)$
$D_{\ell,p}$ $D_{\ell,n}$
$D_{s,p}$ $D_{s,n}$
$\mu(J)/\mu_N$
$\langle J-\Delta J||M_1||J\rangle/\mu_N$
1/2 3/2 5/2 7/2 9/2 11/2 13/2 15/2 17/2
$J$

# E2 moments and transitions

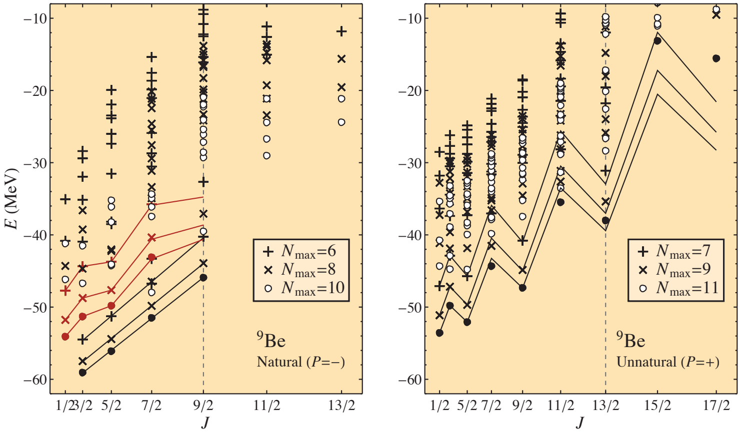


# E2 and M1 moments and transitions



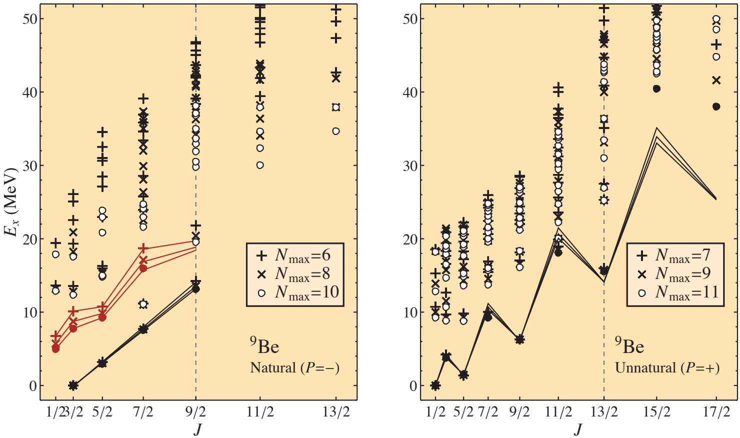
# Convergence with basis space

Absolute binding energy? NO!



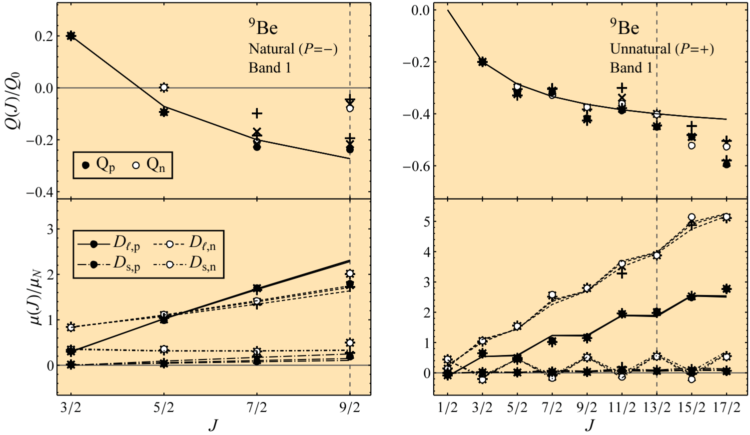
# Convergence with basis space

Absolute binding energy? NO! Excitation within band? ~YES



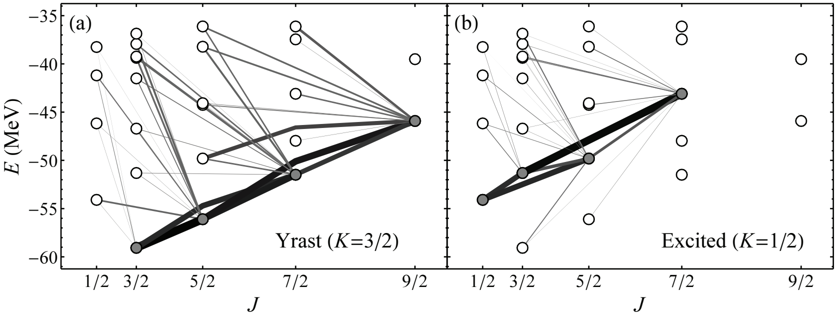
# Convergence with basis space

Absolute $E2$? NO! Ratio of $E2$? ~YES Absolute $M1$? ~YES



# Inter- and Intra-band E2 transtions

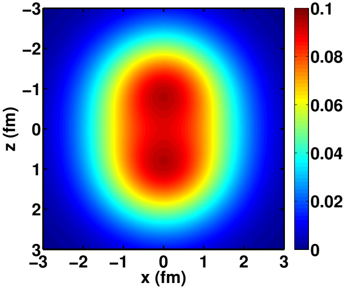
Caprio, Maris, Vary, Smith, IJMPE 24, 1541002 (2015)

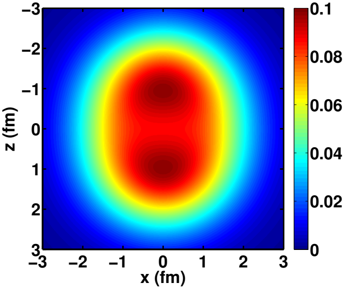



E2 transition strenght between natural (negative) parity states in $^9$Be

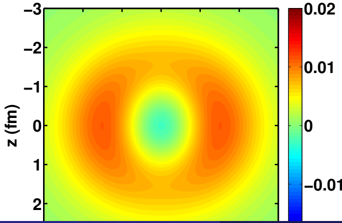
- Transitions within g.s. ($K = 3/2$) and ($K = 1/2$) bands significantly enhanced over typical E2 transition strenght

# One-body density of 9Be ground state $(\frac{3}{2}^-, \frac{1}{2})$




and their difference

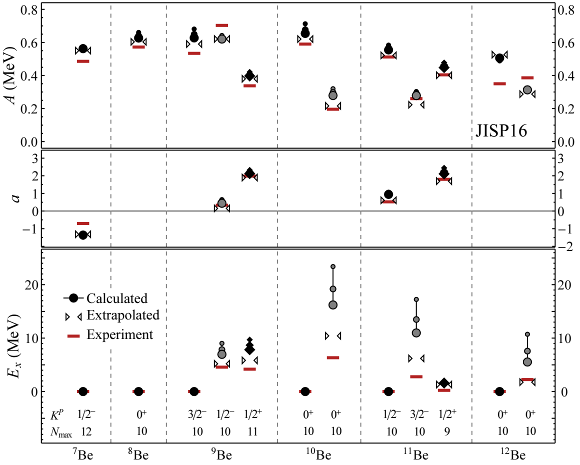



- Relative proton and neutron densities Cockrell, PhD thesis, 2012
- Emergence of $\alpha$ clustering
  - extra neutron appears to be in $\pi$ orbital

# Extraction of band parameters

Caprio, Maris, Vary, Smith, IJMPE 24, 1541002 (2015)

Rotational constant $A$ Coriolis decoupling $a$ Excitation energy $E_x$

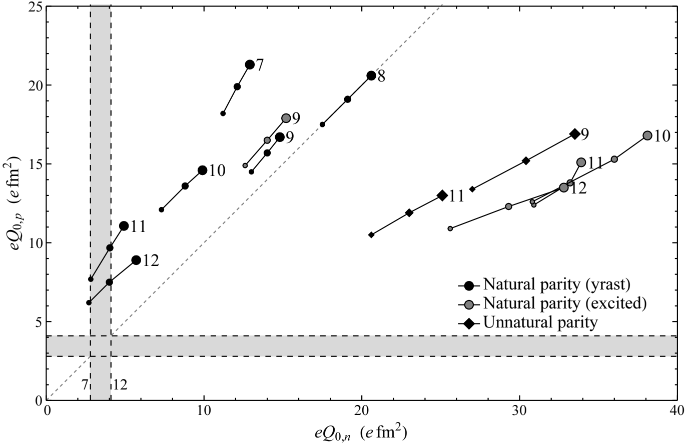


# Convergence of intrinsic quadrupole moments

Caprio, Maris, Vary, Smith, IJMPE 24, 1541002 (2015)

Quadrupole moments? NO! Ratios of $p$ & $n$ moments? ~ YES

Enhanced relative to single-particle strength (Weisskopf)



# Convergence of observables

- Binding energies
  - need extrapolations
  - alternatives for H.O. basis and/or different truncation scheme?
- Excitation energies
  - okay for narrow states (of similar structure as bound state)
  - H.O. basis not suited for broad resonances
  - alternatives for H.O. basis, specifically for resonances?
- Magnetic moments and transitions
  - converge generally rapidly
  - need to add meson-exchange currents
- Quadrupole moments and transitions
  - converge slowly
  - however, ratio's of E2 observables reasonably well converged
  - extrapolations? Odell, Papenbrock and Platter, PRC 93, 044331 (2016)
  - alternatives for H.O. basis and/or different truncation scheme?
- Emergence of rotational structure and clustering