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Ab initio estimation of math xmlns="http://www.w3.org/1998/Math/MathML">mrow>mi >E/mi>mn>2/mn>/mrow>/math> strengths in math xmlns="http://www.w3.org/1998/Math/MathML">mmultiscri pts>mi>Li/mi>mprescripts>/mprescripts>none>/none>m n>8/mn>/mmultiscripts>/math> and its neighbors by normalization to the measured quadrupole moment Mark A. Caprio and Patrick J. Fasano Phys. Rev. C **106**, 034320 — Published 26 September 2022 DOI: 10.1103/PhysRevC.106.034320

## *Ab initio* estimation of *E*2 strengths in <sup>8</sup>Li and its neighbors by normalization to the measured quadrupole moment

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(Dated: September 6, 2022)

For electric quadrupole (E2) observables, which depend on the large-distance tails of the nuclear wave function, *ab initio* no-core configuration interaction (NCCI) calculations converge slowly, making meaningful predictions challenging to obtain. Nonetheless, the calculated values for different E2 matrix elements, particularly those involving levels with closely-related structure (*e.g.*, within the same rotational band) are found to be robustly proportional. This observation suggests that a known value for one observable may be used to determine the overall scale of E2 strengths, and thereby provide predictions for others. In particular, we demonstrate that meaningful predictions for E2 transitions may be obtained by calibration to the groundstate quadrupole moment. We test this approach for well-measured low-lying E2 transitions in <sup>7</sup>Li and <sup>9</sup>Be, then provide predictions for transitions in <sup>8</sup>Li and <sup>9</sup>Li. In particular, we address the  $2^+ \rightarrow 1^+$  transition in <sup>8</sup>Li, for which the reported measured strength exceeds *ab initio* Green's function Monte Carlo (GFMC) predictions by over an order of magnitude.

#### I. INTRODUCTION

Electric quadrupole (*E*2) observables provide key measures of nuclear collective structure [1–3], in particular, rotation and deformation. However, *ab initio* calculations for *E*2 observables are notoriously challenging to obtain [4–6]. Since *E*2 observables are sensitive to the large-distance tails of the nuclear wave function, they are slowly convergent in *ab initio* no-core configuration interaction (NCCI), or no-core shell model (NCSM), approaches [7], which conventionally rely upon an oscillator-basis expansion of the wave function. In practical calculations, the basis for the many-body space must be truncated to finite size. The <sup>15</sup> results can therefore, at best, only approximate the *E*2 predictions which would be obtained
<sup>16</sup> by solving the full (untruncated) many-body problem for a given internucleon interaction.
<sup>17</sup> While one may attempt to improve the many-body calculation by various means (*e.g.*,
<sup>18</sup> Refs. [8–12]) so as to improve convergence of *E*2 observables, the accuracy is nonetheless
<sup>19</sup> severely limited by computational constraints.

We may thus, alternatively, seek indirect ways to circumvent the convergence challenges affecting E2 observables. In particular, the convergence patterns of calculated E2 matrix elements are often strongly correlated [13–18], especially for matrix elements involving states with similar structure. This suggests [14] that, if one E2 matrix element is well-known from experiment (or, in principle, a complementary *ab initio* calculation using an alternative many-body method), a meaningful prediction may then be made for another, correlated E2 matrix element. Calci and Roth [14] use the well-measured E2 strength between the ground state and first excited state, in <sup>6</sup>Li and <sup>12</sup>C, to obtain a prediction for the elusive excited-state quadrupole moment.

<sup>29</sup> Conversely, in the present work, we demonstrate the viability of the ground-state <sup>30</sup> quadrupole moment as a calibration reference by which to generate predictions of E2<sup>31</sup> strengths, through robust *ab initio* NCCI predictions of the dimensionless ratio  $B(E2)/(eQ)^2$ , <sup>32</sup> in which systematic truncations errors in the calculated E2 matrix elements cancel. The <sup>33</sup> ground-state quadrupole moment is well-measured for many nuclei [19], as summarized <sup>34</sup> for *p*-shell nuclides in Fig. 1. Calibration to this observable is subject to the fundamental <sup>35</sup> constraint that the ground state angular momentum must admit a nonvanishing quadrupole <sup>36</sup> moment  $(J \geq 1)$ , as well as practical constraints that measurement must be feasible [25], <sup>37</sup> including that the ground state must be particle-bound.

The case of <sup>8</sup>Li is of particular interest, as an instance in which this approach may be applied to obtain *ab initio* insight, given the anomalously enhanced strength reported for the transition between the 2<sup>+</sup> ground state and 1<sup>+</sup> first excited state of this nuclide. This *E*2 strength has been measured through Coulomb excitation of <sup>8</sup>Li in a radioactive beam experiment, yielding  $B(E2; 2^+ \rightarrow 1^+) = 55(15) e^2 \text{fm}^4$  [21, 26], or, in terms of the Weisskopf single-particle estimate [27],  $\approx 58 \text{ W.u.}$  (The gamma decay lifetime of the 1<sup>+</sup> state instead yields only information on the *M*1 strength [21].) This is among the most enhanced *E*2 transition strengths reported in a *p*-shell nuclide [20–24]. Compare, *e.g.*,  $B(E2; 3/2^- \rightarrow 1/2^-) \approx 10 \text{ W.u.}$  for the analogous (upward) transition from the ground



FIG. 1. Nuclides with measured ground-state quadrupole moments [19] (indicated with the letter "Q") in the p shell. Particle-bound nuclides are designated by name, while brackets indicate a particle-unbound but narrow ( $\leq 1 \text{ keV}$ ) ground-state resonance, and shading indicates stable nuclides. The ground-state angular momentum and parity are given [20–24] (upper right), while slashes serve to exclude those nuclei (with  $J \leq 1/2$ ) for which the ground-state angular momentum does not support a quadrupole moment. The nuclide <sup>8</sup>Li and its neighbors considered in this work are highlighted (dashed circles). Figure adapted from Ref. [18].

<sup>47</sup> state of neighboring <sup>7</sup>Li [20], or  $B(E2; 3/2^- \rightarrow 5/2^-) \approx 42$  W.u. similarly in neighboring <sup>48</sup> <sup>9</sup>Be [24].

<sup>49</sup> However, Green's function Monte Carlo (GFMC) calculations [28] give a predicted <sup>50</sup> strength nearly two orders of magnitude smaller, at  $0.83(7) e^2 \text{fm}^4$  [28]. Moreover, we note <sup>51</sup> that such enhancement in <sup>8</sup>Li would be particularly remarkable, given that it cannot be <sup>52</sup> explained in terms of in-band rotational collectivity, while the aforementioned transitions <sup>53</sup> in neighboring <sup>7</sup>Li and <sup>9</sup>Be are ostensibly rotational in nature [17]. Even if the 2<sup>+</sup> ground <sup>54</sup> state is taken to be a K = 2 rotational band head, this band would have no J = 1 member. <sup>55</sup> We first establish the expected form for the correlation between B(E2) and quadrupole <sup>56</sup> moment observables, through the dimensionless ratio  $B(E2)/(eQ)^2$  (Sec. II), and demon-<sup>57</sup> strate the robust convergence of this ratio for experimentally well-measured E2 transition <sup>58</sup> strengths, between the ground state and first excited state (of the same parity), in <sup>7</sup>Li <sup>59</sup> and <sup>9</sup>Be (Sec. III). We then return to the anomalous 2<sup>+</sup>  $\rightarrow$  1<sup>+</sup> transition in <sup>8</sup>Li and other <sup>60</sup> unmeasured E2 strengths to low-lying states in <sup>8</sup>Li and <sup>9</sup>Li (Sec. IV).

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### **II. DIMENSIONLESS RATIO**

The E2 reduced transition probability depends upon the square of a reduced matrix
 element of the E2 operator, as

$$B(E2; J_i \to J_f) \propto |\langle J_f \| Q_2 \| J_i \rangle|^2, \tag{1}$$

<sup>64</sup> while the quadrupole moment, originally defined in terms of the stretched matrix element <sup>65</sup>  $\langle JJ | Q_{2,0} | JJ \rangle$ , is simply proportional to a reduced matrix element, as

$$eQ(J) \propto \langle J \| Q_2 \| J \rangle. \tag{2}$$

<sup>66</sup> The sensitivity of each observable to the large-distance properties of the nuclear wave func-<sup>67</sup> tion arises from the  $r^2$  dependence of the E2 operator [29],  $Q_{2\mu} = \sum_{i \in p} er_i^2 Y_{2\mu}(\hat{\mathbf{r}}_i)$ , where <sup>68</sup> the summation runs over the (charged) protons. The ratio

$$\frac{B(E2)}{(eQ)^2} \propto \left| \frac{\langle J_f \| Q_2 \| J_i \rangle}{\langle J \| Q_2 \| J \rangle} \right|^2 \tag{3}$$

<sup>69</sup> is dimensionless, and involves like powers of reduced matrix elements of the *E*2 operator in <sup>70</sup> the numerator and denominator. We thus have reason to hope for at least partial cancellation <sup>71</sup> of the error arising in these matrix elements due to truncation of the nuclear wave functions.

#### III. ILLUSTRATION FOR <sup>7</sup>Li AND <sup>9</sup>Be

In the NCCI approach, the true results of solving the many-body problem in the full manyray body space would be obtained if the full, infinite oscillator basis could be used. However, rs for finite calculations, results depend upon the subspace spanned by the truncated basis. r6 Thus they depend both upon the maximum number  $N_{\text{max}}$  of oscillator excitations allowed r7 within the configurations making up the many-body basis, and upon the oscillator length r8 of the underlying single-particle states (or, equivalently, the oscillator parameter  $\hbar\omega$  [29]). r9 Convergence is recognized when the calculated results become insensitive to increases in so  $N_{\text{max}}$  and to variation in  $\hbar\omega$  (see, *e.g.*, Refs. [4, 5, 17]).

Let us first consider the convergence of the calculated  $3/2^- \rightarrow 1/2^- E2$  strength for <sup>82</sup> <sup>7</sup>Li, shown in Fig. 2(a), as obtained using the Daejeon16 internucleon interaction [30]. This <sup>83</sup> interaction is based on the two-body part of the Entem-Machleidt N<sup>3</sup>LO chiral effective <sup>84</sup> field theory ( $\chi$ EFT) interaction [31], softened via a similarity renormalization group (SRG) <sup>85</sup> transformation [32] so as to provide comparatively rapid convergence, and then adjusted <sup>86</sup> via a phase-shift equivalent transformation to better describe nuclei with  $A \leq 16$  while <sup>87</sup> still maintaining rapid convergence. Calculations are carried out using the NCCI code <sup>88</sup> MFDn [33–35]. (Comprehensive plots and tabulations of calculated observables, as functions <sup>89</sup> of  $N_{\text{max}}$  and  $\hbar\omega$ , are provided in the Supplemental Material [36].)

The values along each curve in Fig. 2 represent the results of calculations carried out with <sup>90</sup> the same basis truncation  $N_{\text{max}}$  (from short dashes for  $N_{\text{max}} = 4$  to solid lines for  $N_{\text{max}} = 16$ ) <sup>92</sup> and differing  $\hbar\omega$ . While there is perhaps some tendency towards flattening of these curves <sup>93</sup> with respect to  $\hbar\omega$  ("shouldering") and compression of successive curves with respect to <sup>94</sup>  $N_{\text{max}}$ , the calculated values are still steadily increasing with increasing  $N_{\text{max}}$ . At best, we <sup>95</sup> might crudely estimate the true value which would be obtained for the given internucleon <sup>96</sup> interaction in the full, untruncated many-body space.

<sup>97</sup> A similar convergence pattern is found for the calculated  $3/2^-$  ground state quadrupole <sup>98</sup> moment [Fig. 2(d)], where, however, the curves are inverted due to the negative sign on the <sup>99</sup> quadrupole moment. (For further discussion of the convergence of this and other quadrupole <sup>100</sup> moments in NCCI calculations, see Ref. [18].) With each increment in  $N_{\text{max}}$ , the relative <sup>101</sup> (fractional) change between calculated values of the quadrupole moment is smaller than for <sup>102</sup> the B(E2). This is to be expected, as the quadrupole moment is simply proportional to a



FIG. 2. Convergence of *ab initio* NCCI calculated observables for <sup>7</sup>Li: (top) the  $3/2^- \rightarrow 1/2^- E2$ strength, (middle) the electric quadrupole moment of the  $3/2^-$  ground state, and (bottom) the dimensionless ratio  $B(E2)/(eQ)^2$  constructed from the preceding two observables. Results are shown for the (left) Daejeon16, (center) JISP16, and (right) LENPIC interactions. When calibrated to the experimental quadrupole moment, the ratio provides a prediction for the absolute B(E2) (scale at right). Calculated values are shown as functions of the basis parameter  $\hbar\omega$ , for successive even value of  $N_{\text{max}}$  (increasing symbol size and longer dashing), from  $N_{\text{max}} = 4$  (short dashed curves) to 16 (solid curves). For comparison, experimental values [19, 20] (squares), GFMC AV18+IL7 predictions [28] (crosses), and the rotational ratio (asterisk) are also shown.

<sup>103</sup> matrix element of the E2 operator, while the B(E2) is proportional to the square of such a <sup>104</sup> matrix element, and (as in elementary error analysis) squaring a quantity doubles relative <sup>105</sup> changes in that quantity. However, one may again at best attempt a crude estimate of the <sup>106</sup> value which would be obtained in the full, untruncated many-body space.

In <sup>7</sup>Li, both the *E*2 strength and the quadrupole moment are known experimentally, with measured values of  $B(E2; 3/2^- \rightarrow 1/2^-) = 8.3(5) e^2 \text{fm}^4$  [20] and  $Q(3/2^-) =$ 



FIG. 3. Calculated excitation energies of low-lying states in (a) <sup>7</sup>Li and (b) <sup>9</sup>Be, with angular momentum and parity as indicated at bottom, as obtained with the Daejeon16 interaction. Calculated values are shown at fixed  $\hbar \omega = 20$  MeV and varying  $N_{\text{max}}$  (increasing symbol size), from  $N_{\text{max}} = 4$ to the maximum value indicated (at top). Experimental energies [20, 21] are shown (horizontal line and error band) where available, as are the GFMC AV18+IL7 predictions [28] (crosses) (see Table III of Ref. [37]).

 $_{109}$  -4.00(3) fm<sup>2</sup> [19, 20] (squares in Fig. 2). While the NCCI calculated values for both the  $_{110}$  B(E2) [Fig. 2(a)] and quadrupole moment [Fig. 2(d)] are increasing in the general direc-111 tion of the experimental result, these poorly-converged results do not permit meaningful, 112 quantitative comparison.

However, let us now take the dimensionless ratio of the form defined in (3) for these 113 observables, namely,  $B(E2; 3/2^- \rightarrow 1/2^-)/[eQ(3/2^-)]^2$ , with the result shown in Fig. 2(g). 114 We find a near complete elimination of the  $\hbar\omega$  dependence, at the higher  $N_{\rm max}$  shown, as 115 well as a radical compression of the curves for successive  $N_{\text{max}}$ . Calibrating to the known 116 ground-state quadrupole moment [19] gives the scale shown at far right [Fig. 2 (bottom)]. An 117 estimated ratio of  $B(E2; 3/2^- \rightarrow 1/2^-)/[eQ(3/2^-)]^2 \approx 0.50$  yields  $B(E2; 3/2^- \rightarrow 1/2^-) \approx 0.50$ 118  $8 e^2 \text{fm}^4$ . The predicted ratio  $B(E2)/(eQ)^2$  is consistent, to within uncertainties, with the 119 <sup>120</sup> experimental ratio of 0.52(3), and the resulting B(E2) is similarly within uncertainties of <sup>121</sup> the experimental strength.

From a physical viewpoint, the close-lying  $3/2^-$  ground state and  $1/2^-$  excited state <sup>123</sup> in <sup>7</sup>Li are interpreted as members of a K = 1/2 rotational band [38], where the energy <sup>124</sup> order is inverted due to Coriolis staggering [3]. For context, the calculated and experi-<sup>125</sup> mental excitation energies of the yrast levels are shown in Fig. 3(a) (see also Fig. 3 of <sup>126</sup> Ref. [17] and Fig. 2 of Ref. [11] for more extensive calculated level schemes, of the mirror <sup>127</sup> nuclide <sup>7</sup>Be, obtained with the same Daejeon16 interaction). The rotational model yields <sup>128</sup>  $B(E2; 3/2_{K=1/2} \rightarrow 1/2_{K=1/2})/[eQ(3/2_{K=1/2})]^2 \approx 0.497$ , indicated by the asterisk in Fig. 2(g). <sup>129</sup> We are thus seeing close consistency between *ab initio* theory and experiment, both of which <sup>130</sup> are well-explained by a simple rotational picture [13].

To explore the dependence upon internucleon interaction, let us consider the results for 132 these same observables, but from calculations based on the JISP16 [Fig. 2 (center)] and 133 LENPIC Fig. 2 (right)] internucleon interactions. The phenomenological JISP16 interac-134 tion [39] is obtained by *J*-matrix inverse scattering from nucleon-nucleon scattering data, 135 and, like Daejeon16, adjusted via a phase-shift equivalent transformation to better describe 136 nuclei with  $A \leq 16$ . The LENPIC interaction [40, 41] is a modern chiral EFT interaction (we 137 specifically take the two-body part, at N<sup>2</sup>LO, with a semi-local coordinate-space regulator 138 of length scale R = 1 fm, and, for purposes of illustration, use the bare interaction with no 139 SRG transformation).

For the B(E2) itself, there is at best minimal suggestion of convergence, or shouldering, 141 in the JISP16 results [Fig. 2(b)], and essentially no sign of convergence in the LENPIC 142 results [Fig. 2(c)]. The same may be said for the computed quadrupole moments [Fig. 2(e,f)]. 143 Nonetheless, taking the dimensionless ratio  $B(E2)/(eQ)^2$  [Fig. 2(h,i)] again leads to a rapidly 144 convergent quantity, from which the  $\hbar\omega$  dependence has largely been eliminated, and the 145 changes with successive  $N_{\text{max}}$  rapidly decrease. The resulting values for the ratio, as obtained 146 with these interactions, is closely consistent both with that obtained from the Daejeon16 147 interaction [Fig. 2(g)] and with experiment.

Predictions for this same quadrupole moment and transition matrix element in <sup>7</sup>Li have previously been reported [28] from *ab initio* Green's function Monte Carlo (GFMC) [37] calculations, based on the Argonne  $v_{18}$  (AV18) two-nucleon [42] and Illinois-7 (IL7) threenucleon [43] potentials. These predictions, shown as crosses in Fig. 2 (left), are subject to Monte Carlo statistical errors, so the calculational uncertainties are of a qualitatively different nature from those entering into the NCCI calculations. In particular, the GFMC calulated values for the *E*2 transition strength [Fig. 2(a)] and quadrupole moment [Fig. 2(d)] may meaningfully be compared directly with experiment, without taking a ratio to can-



FIG. 4. Calculated ratios of the form  $B(E2)/(eQ)^2$ , for excitation to low-lying states in <sup>7</sup>Li and <sup>9</sup>Be, obtained with the Daejeon16, JISP16, and LENPIC interactions (from left to right, for each transition). Calculated values are shown at fixed  $\hbar\omega = 20$  MeV and varying  $N_{\text{max}}$  (increasing symbol size), from  $N_{\text{max}} = 4$  to the maximum value indicated (at top). When calibrated to the experimental quadrupole moment [19], this ratio provides an estimate for the absolute B(E2) (scale at right). Experimental results [19–21] are shown (horizontal line and error band) where available, as are the GFMC AV18+IL7 predictions [28] (crosses) and rotational ratios (asterisks).

<sup>156</sup> cel truncation errors, and we see agreement within uncertainties in both cases. Nonethe-<sup>157</sup> less, for comparison with the NCCI results, we may recast these GFMC results as a ratio <sup>158</sup>  $B(E2)/(eQ)^2$  [cross in Fig. 2(g)], where we find consistency with experiment (again), but <sup>159</sup> now also with the NCCI predictions for the ratio.

To provide for convenient comparison across calculations and (in the following discus-161 sion) transitions, we take a "slice" through these NCCI results in Fig. 4(a), which shows 162 convergence with  $N_{\text{max}}$  at fixed  $\hbar\omega$  (chosen as  $\hbar\omega = 20$  MeV, based on the approximate lo-163 cation of the variational energy minimum for the ground state, although this location varies 164 somewhat by nuclide and interaction). We may again readily compare the NCCI results 165 with experiment (horizontal lines and shaded error bands), GFMC AV18+IL7 predictions



FIG. 5. Convergence of the *ab initio* NCCI calculated dimensionless ratio  $B(E2)/(eQ)^2$ , for <sup>9</sup>Be, constructed from the  $3/2^- \rightarrow 5/2^- E2$  strength and the electric quadrupole moment of the  $3/2^-$  ground state. Results are shown for the Daejeon16 interaction. When calibrated to the experimental quadrupole moment, the ratio provides a prediction for the absolute B(E2) (scale at right). Calculated values are shown as functions of the basis parameter  $\hbar\omega$ , for successive even value of  $N_{\text{max}}$  (increasing symbol size and longer dashing), from  $N_{\text{max}} = 4$  (short dashed curves) to 10 (solid curves). For comparison, the experimental ratio [19, 21] (square), GFMC AV18+IL7 prediction [28] (cross), and rotational ratio (asterisk) are also shown.

<sup>166</sup> (crosses), and the rotational model (asterisks), where applicable.

In <sup>9</sup>Be, the *E*2 transition from the  $3/2^{-}$  ground state to the  $5/2^{-}$  excited state (a narrow resonance just above the neutron threshold, with a width of  $\approx 0.8 \text{ keV}$  [20]) is interpreted as an in-band transition within the ground-state (K = 3/2) rotational band [38]. For context, calculated and experimental excitation energies of the (normal-parity [44]) yrast levels of the including the J = 3/2, 5/2, and 7/2 members of the ground state K = 3/2 band and transition K = 1/2 band head, are shown in Fig. 3(b) (see also Fig. 1 of Ref. [17] for a more extensive calculated level scheme, obtained with the same Daejeon16 interaction).

The dimensionless ratio  $B(E2)/(eQ)^2$ , as obtained with the Daejeon16 interaction, is 175 shown in Fig. 5, and similar results are obtained with the other two interactions consid-176 ered above, as summarized in Fig. 4(b). Again, taking the dimensionless ratio largely 177 eliminates the  $\hbar\omega$  dependence of the results and yields rapid convergence with respect 178 to  $N_{\text{max}}$ . Calibrating to the known ground-state quadrupole moment [19] gives the scale 179 shown at right. An estimated ratio of  $B(E2; 3/2^- \rightarrow 5/2^-)/[eQ(3/2^-)]^2 \approx 1.3-1.4$  yields  $_{180} B(E2; 3/2^- \rightarrow 5/2^-) \approx 36-39 e^2 \text{fm}^4$ . The NCCI results for this ratio (with all three inter- $_{181}$  actions) lie just below the uncertainty ranges for the experimental ratio (square) and for  $_{182}$  the GFMC AV18+IL7 predictions (cross), and just above the ratio of  $B(E2; 3/2_{K=3/2}) \rightarrow$  $_{183} 5/2_{K=3/2})/[eQ(3/2_{K=3/2})]^2 \approx 1.279$  for an ideal rotational description (asterisk).

The strength of any interband E2 transition to the  $1/2^-$  band head is experimentally unknown [21]. However, the present NCCI calculations give a ratio  $B(E2)/(eQ)^2$  which is essentially vanishing on the scale of Fig. 4(d). The calculated ratios  $B(E2; 3/2^- \rightarrow$  $1/2^-)/[eQ(3/2^-)]^2 \leq 0.005$  suggest  $B(E2; 3/2^- \rightarrow 1/2^-) \leq 0.2 e^2 \text{fm}^4$ . In a rotational description, the interband E2 strength depends upon the interband intrinsic E2 matrix element [1–3], and a limit on the ratio  $B(E2)/(eQ)^2$  may be translated, through appropriate Clebsch-Gordan factors, into a limit on the ratio of in-band and interband intrinsic matrix elements.

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#### IV. PREDICTIONS FOR <sup>8</sup>Li AND <sup>9</sup>Li

Returning to the  $2^+ \rightarrow 1^+$  transition in <sup>8</sup>Li, the NCCI calculations for the relevant observables are shown in Fig. 6. For context, calculated and experimental excitation energies of low-lying levels in <sup>8</sup>Li are shown in Fig. 7(a). We again compare results obtained for the Daejeon16 [Fig. 6(a)], JISP16 [Fig. 6(b)], and LENPIC [Fig. 6(c)] interactions.

Focusing first on the Daejeon16 results [Fig. 6(a)], we see that taking the dimensionless <sup>201</sup> Focusing first on the Daejeon16 results [Fig. 6(a)], we see that taking the dimensionless <sup>202</sup> ratio  $B(E2; 2^+ \to 1^+)/[eQ(2^+)]^2$  rapidly eliminates the  $\hbar\omega$  and  $N_{\rm max}$  dependence, at the <sup>203</sup> scale shown, even for modest  $N_{\rm max}$ . Calibrating to the known  $Q(2^+) = +3.14(2)$  fm<sup>2</sup> [19] <sup>204</sup> yields the scale at far right. A ratio of  $\approx 0.18$ , taken in conjunction with this quadrupole <sup>205</sup> moment, yields an estimated  $B(E2; 2^+ \to 1^+) \approx 1.8 e^2 \text{fm}^4$ .

For the JISP16 interaction [Fig. 6(b)], the dimensionless ratio exhibits greater  $\hbar\omega$  de-<sup>207</sup> pendence than found for Daejeon16 [Fig. 6(a)], especially for lower  $N_{\text{max}}$ . Nonetheless, it <sup>208</sup> appears to robustly converge towards a result,  $B(E2; 2^+ \rightarrow 1^+)/[eQ(2^+)]^2 \approx 0.10$ , in this <sup>209</sup> case lower by nearly a factor of two than obtained for Daejeon16.



FIG. 6. Convergence of the *ab initio* NCCI calculated dimensionless ratio  $B(E2)/(eQ)^2$ , for <sup>8</sup>Li, constructed from the  $2^+ \rightarrow 1^+ E2$  strength and the electric quadrupole moment of the  $2^+$  ground state. Results are shown for the (a) Daejeon16, (b) JISP16, and (c) LENPIC interactions. When calibrated to the experimental quadrupole moment, the ratio provides a prediction for the absolute B(E2) (scale at right). Calculated values are shown as functions of the basis parameter  $\hbar\omega$ , for successive even value of  $N_{\rm max}$  (increasing symbol size and longer dashing), from  $N_{\rm max} = 4$  (short dashed curves) to 14 (solid curves). For comparison, the GFMC AV18+IL7 prediction [28] (crosse) is shown, while the experimental ratio [19, 21], corresponding to the reported E2 strength of  $55(15) e^2 \text{fm}^4$  [26], lies off scale.

For the LENPIC interaction [Fig. 6(c)], taking the dimensionless ratio tames the  $\hbar\omega$ <sup>211</sup> dependence, indeed, more effectively than for JISP16 [Fig. 6(b)]. There is still a slow but <sup>212</sup> steady increase with  $N_{\text{max}}$  over much of the  $\hbar\omega$  range. Nonetheless, with this caveat, the <sup>213</sup> calculated ratio is again in the vicinity of 0.10.<sup>1</sup>

Thus, as summarized in Fig. 8(a), the NCCI predictions show the ratio  $B(E2)/(eQ)^2$ 215 to depend upon the choice of interaction, varying within the range  $\approx 0.1-0.2$ . By way of 216 comparison, GFMC calculation [28] gives  $B(E2; 2^+ \rightarrow 1^+) = 0.83(7) e^2 \text{fm}^4$  and  $Q(2^+) =$ 217 +3.3(1) fm<sup>2</sup>, which, recast as a ratio, yield  $B(E2; 2^+ \rightarrow 1^+)/[eQ(2^+)]^2 = 0.076(8)$ , similar 218 in scale to and marginally below these NCCI estimates.

That the *ab initio* predictions for the  $2^+ \rightarrow 1^+$  transition, and in particular for the 220 ratio to the squared quadrupole moment, show a greater dependence upon the internucleon

<sup>1</sup> The earlier NCCI calculations of Maris *et al.* [45], based on the chiral N<sup>3</sup>LO two-nucleon interaction of Entem and Machleidt [31], together with the N<sup>2</sup>LO three-nucleon interaction of Navrátil [46], carried out using a basis with  $N_{\text{max}} = 8$  and  $\hbar \omega = 13$  MeV, and calculated with an Okubo-Lee-Suzuki [47, 48] renormalized effective interaction, give  $Q(2^+) = 2.648 \text{ fm}^2$  and  $B(E2; 2^+ \to 1^+) = 0.714 e^2 \text{fm}^4$ , similarly yielding a ratio of  $B(E2; 2^+ \to 1^+)/[eQ(2^+)]^2 \approx 0.10$ .



FIG. 7. Calculated excitation energies of low-lying states in (a) <sup>8</sup>Li and (b) <sup>9</sup>Li, with angular momentum and parity as indicated at bottom, as obtained with the Daejeon16 interaction. Calculated values are shown at fixed  $\hbar \omega = 20 \text{ MeV}$  and varying  $N_{\text{max}}$  (increasing symbol size), from  $N_{\text{max}} = 4$  to the maximum value indicated (at top). Experimental energies [21] are shown (horizontal line and error band) where available, as are the GFMC AV18+IL7 predictions [28] (crosses) (see Table III of Ref. [37]).

<sup>221</sup> interaction than found above (Sec. III) for the in-band rotational transitions in <sup>7</sup>Li and <sup>9</sup>Be is <sup>222</sup> perhaps not surprising. One may take the perspective that the E2 ratio is not "constrained" <sup>223</sup> by the symmetry considerations which apply to in-band transitions in an axially symmetric 224 rotor or, perhaps, an Elliott SU(3) rotor [38, 49, 50]. If the  $2^+ \rightarrow 1^+$  transition is taken to be an interband transition, rather, it is sensitive to the detailed microscopic structure of 225 rotational intrinsic states. More generally, the transition involved is (predicted to be) a weak 226 ("noncollective") transition, which might be expected to be sensitive, *e.g.*, in a shell model 227 picture, to admixtures of different *p*-shell configurations favored by the different interactions. 228 However, taken in conjunction with the known  $Q(2^+) = +3.14(2) \text{ fm}^2$  [19], these *ab initio* 229 results are all consistent with a modest strength of  $\approx 1-2 e^2 \text{fm}^4$  for the  $2^+ \rightarrow 1^+$  transition, 230 more than an order of magnitude smaller than the experimental value of  $55(15) e^2 \text{fm}^4$  [21, 26]. 231

232 It is thus of particular interest to obtain confirmation of this reported strength.

It is interesting to contrast the results for this  $2^+ \rightarrow 1^+$  transition in <sup>8</sup>Li with the results for the ostensibly in-band  $2^+ \rightarrow 3^+$  transition, shown in Fig. 8(b). In a rotational description, the  $3^+$  second excited state (a narrow resonance at 2.2 MeV, just above the



FIG. 8. Calculated ratios of the form  $B(E2)/(eQ)^2$ , for excitation to low-lying states in <sup>8</sup>Li and <sup>9</sup>Li, obtained with the Daejeon16, JISP16, and LENPIC interactions (from left to right, for each transition). Calculated values are shown at fixed  $\hbar \omega = 20$  MeV and varying  $N_{\text{max}}$  (increasing symbol size), from  $N_{\text{max}} = 4$  to the maximum value indicated (at top). When calibrated to the experimental quadrupole moment [19], this ratio provides an estimate for the absolute B(E2) (scale at right). Experimental results [19, 21] are shown (horizontal line and error band) where available (the <sup>8</sup>Li 2<sup>+</sup>  $\rightarrow$  1<sup>+</sup> transition strength lies off scale), as are the GFMC AV18+IL7 predictions [28] (crosses) and rotational ratios (asterisks).

<sup>236</sup> neutron separation threshold) is naturally taken as a member of the K = 2 ground state <sup>237</sup> band. Experimentally, only the M1 partial decay width is known [21], from a <sup>7</sup>Li $(n, \gamma)$ <sup>238</sup> measurement [51], while a Coulomb excitation measurement for the E2 strength would <sup>239</sup> require neutron detection. The NCCI calculations, as obtained with the three different <sup>240</sup> interactions, suggest ratios  $B(E2; 2^+ \rightarrow 3^+)/[eQ(2^+)]^2$  in the range  $\approx 0.7$ –1.0, with the <sup>241</sup> GFMC prediction [28] coming in at the low end of this range, and the rotational ratio of <sup>242</sup>  $\approx 0.609$  coming lower still. In conjunction with the known quadrupole moment, the NCCI <sup>243</sup> calculated ratios yield a comparatively collective  $B(E2; 2^+ \rightarrow 3^+)$  of  $\approx 7$ –10  $e^2$ fm<sup>4</sup>.

We conclude with NCCI predictions for the unmeasured E2 strengths from the  $3/2^{-1}$ 

<sup>245</sup> ground state of <sup>9</sup>Li to the first two excited states [21]. The only excited state below the <sup>246</sup> neutron threshold is a  $1/2^{-}$  state at  $\approx 2.7 \,\text{MeV}$ , while a resonance at  $\approx 4.3 \,\text{MeV}$ , just <sup>247</sup> above the neutron threshold, has tentative  $(5/2^{-})$  assignment. This low-lying spectrum is <sup>248</sup> consistent with the level ordering obtained in the present NCCI calculations. Calculated <sup>249</sup> and experimental excitation energies are shown in Fig. 7(b).

The NCCI predictions for the dimensionless ratio  $B(E2; 3/2^- \rightarrow 1/2^-)/[eQ(3/2^-)]^2$ , shown in Fig. 8(c), are robustly converged with respect to basis truncation. The ratio is found to depend modestly upon interaction, within the range  $\approx 0.5-0.6$ . Calibrating to the known ground-state quadrupole moment [19] yields strengths, depending upon interaction, in the range  $B(E2; 3/2^- \rightarrow 1/2^-) \approx 4.6-5.5 e^2 \text{fm}^4$ . The GFMC AV18+IL7 predictions [28], recast as a ratio, give 0.64(6), which is roughly consistent with the ratios found in the NCCI calculations. However, on an absolute scale, the GFMC calculated  $257 Q(3/2^-) = -2.3(1) \text{ fm}^2$  underpredicts the experimental quadrupole moment by  $\approx 24\%$ , and and 258 the calculated  $B(E2; 3/2^- \rightarrow 1/2^-) = 3.40(17) e^2 \text{fm}^4$  is thus correspondingly lower than the above estimates.

In a rotational description, it is not a priori obvious whether this transition should <sup>261</sup> be interpreted as an in-band transition within a Coriolis-staggered K = 1/2 band, as in <sup>262</sup> <sup>7</sup>Li (Sec. III), or an interband transition between K = 3/2 ground state and K = 1/2<sup>263</sup> excited band heads. The former interpretation would give an expected rotational ratio of <sup>264</sup>  $B(E2; 3/2_{K=1/2} \rightarrow 1/2_{K=1/2})/[eQ(3/2_{K=1/2})]^2 \approx 0.497$ , as above for <sup>7</sup>Li, while in the latter <sup>265</sup> case the rotational prediction would depend on the ratio of interband and in-band intrinsic <sup>266</sup> matrix elements. The *ab initio* results are roughly consistent with the K = 1/2 in-band <sup>267</sup> interpretation.

For the transition to the  $5/2^-$  state, the NCCI calculations, shown in Fig. 8(d), give  $B(E2; 3/2^- \rightarrow 5/2^-)/[eQ(3/2^-)]^2 \approx 0.01-0.02$ , depending upon choice of interaction, yield-  $B(E2; 3/2^- \rightarrow 5/2^-)/[eQ(3/2^-)]^2 \approx 0.01-0.2 e^2 \text{fm}^4$ . The *ab initio* predicted  $B(E2; 3/2^- \rightarrow 5/2^-) \approx 0.1-0.2 e^2 \text{fm}^4$ . The *ab initio* predicted  $B(E2; 3/2^- \rightarrow 5/2^-) \approx 0.1-0.2 e^2 \text{fm}^4$ . The *ab initio* predicted  $B(E2; 3/2^- \rightarrow 5/2^-) \approx 0.1-0.2 e^2 \text{fm}^4$ . The *ab initio* predicted  $B(E2; 3/2_{K=1/2})/[eQ(3/2_{K=1/2})]^2 \approx 0.213$ , or within a K = 3/2 band built on the ground state,  $B(E2; 3/2_{K=3/2} \rightarrow 5/2_{K=3/2})/[eQ(3/2_{K=3/2})]^2 \approx 1.279$ .

#### V. CONCLUSION

Although meaningful, converged predictions for E2 observables are elusive in *ab initio* NCCI calculations, calculated E2 observables are correlated, presumably due to their common dependence on the truncation of the long-distance tails of the wave functions. For the ground-state quadrupole moment and low-lying transitions, we demonstrate that much of this systematic truncation error cancels out in dimensionless ratios of the form  $B(E2)/(eQ)^2$ , allowing robust predictions to be obtained. Calibrating to the known groundstate quadrupole moment then provides an E2 strength estimate on an absolute scale.

For the rotational in-band transitions in <sup>7</sup>Li and <sup>9</sup>Be, there is general agreement, in the 283  $B(E2)/(eQ)^2$  ratios, between the predictions obtained across several choices for the internu-284 cleon interaction. These calculated values, like the experimental ratios and GFMC predic-285 tions, are approximately consistent with the simple axial rotor model, and calibrating to the 286 ground-state quadrupole moment reproduces the experimentally observed E2 enhancement. 287 For the  $2^+ \rightarrow 1^+$  transition in <sup>8</sup>Li, which is not naturally interpreted as a rotational in-band 288 transition, robust *ab initio* predictions are made for the ratio  $B(E2)/(eQ)^2$ , showing mod-289 est dependence on the choice of internucleon interaction, and reinforcing the severe tension 290 between *ab initio* theory [28] and experiment [21, 26] for this transition. Finally, we provide 291 <sup>292</sup> robust ab initio predictions for the ratio  $B(E2)/(eQ)^2$ , and thus, by normalization to the  $_{293}$  experimental ground state quadrupole moment, estimates for unmeasured E2 strengths to <sup>294</sup> the low-lying  $3^+$  resonance of <sup>8</sup>Li and to low-lying states of <sup>9</sup>Li.

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#### ACKNOWLEDGMENTS

We thank Tan Ahn, Samuel L. Henderson, Pieter Maris, and Anna E. McCoy for valuable discussions, James P. Vary, Ik Jae Shin, and Youngman Kim for sharing illuminating results on ratios of observables, and Colin V. Coane, Jakub Herko, and Zhou Zhou for comments on the manuscript. This material is based upon work supported by the U.S. Department of Energy, Office of Science, under Award No. DE-FG02-95ER40934. This research used resources of the National Energy Research Scientific Computing Center (NERSC), a DOE Office of Science User Facility supported by the Office of Science of the U.S. Department of Energy <sup>303</sup> under Contract No. DE-AC02-05CH11231, using NERSC award NP-ERCAP0020422.

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