COMMENTS

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Comment on "Large-space shell-model calculations for light nuclei"

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In a recent publication Zheng, Vary, and Barrett reproduced the negative quadrupole moment of ^{6}Li and the low-lying positive-parity states of ^{5}He by using a no-core shell model. In this Comment we question the meaning of these results by pointing out that the model used is inadequate for reproducing these properties.

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Recently, Zheng, Vary, and Barrett have published a number of no-core shell-model calculations for light nuclei in a series of papers; see [1] and references therein. By reproducing a vast number of data, they have demonstrated the viability and overall validity of this ambitious fundamental approach. In this Comment we would like to point out that in one respect this approach is not realistic: in treating few-body dynamics in the asymptotic region of the configuration space. Wave-function asymptotics matters for states that lie near or over the breakup thresholds, and the results for these states should be viewed with extreme caution. This shortcoming of the (noncontinuum) shell-model approach is not self-evident; it is only revealed when viewed from the perspective of the complementary cluster-model approach, which treats the few-body dynamics properly.

In their recent article [1] Zheng, Vary, and Barrett presented results for two long-standing problems of light nuclei. Namely, they reproduced the negative quadrupole moment of ^{6}Li and found the previously predicted low-lying positive-parity states of ^{5}He. We shall, however, show that these results hinge on the treatment of the asymptotic few-body dynamics and, in this respect, the shell-model approach used is inadequate. We first discuss the quadrupole moment of ^{6}Li and then the positive-parity states of ^{5}He.

The experimental value of the ^{6}Li quadrupole moment is -0.083 e fm^2 [2]. It is very difficult to reproduce this negative value. The failed attempts to reproduce it include variational three-body calculations [3], the hyperspherical harmonics expansion method [4], the Faddeev approach [5], and a large-space six-body $\alpha+p+n$ three-cluster model [6]. All these calculations gave positive values for Q, in the 0.2–0.6 e fm^2 range. In Ref. [7] it was claimed that a three-cluster model can reproduce the negative quadrupole moment of ^{6}Li if the full six-body antisymmetrization is properly taken into account. This claim was, however, disputed [6], and the result was shown to arise from a restriction on the model space (see also [8]). These macroscopic and microscopic $\alpha+p+n$ calculations revealed that the value of the ^{6}Li quadrupole moment results from a delicate balance between the contributions coming from configurations of different angular momenta in the p-n and α-(pn) relative motions [6,5]. This indicates that, for Q to be reliable, the p-n and α-(pn) dynamics must be described correctly.

In Ref. [1] the model produces $Q=-0.116$ e fm^2. However, in Table I of Ref. [1] we can see that the ground-state binding energy of ^{6}Li is incompatible with those of the deuteron and of the α particle. As a consequence, the model ^{6}Li seems to be unstable against the $\alpha+d$ breakup by 0.21 MeV, in sharp contrast with reality. (The ground state of ^{6}Li is below the $\alpha+d$ threshold by 1.475 MeV [2].) The wave function of ^{6}Li carries information on these aspects in its projection onto the product of the intrinsic wave functions of α and d. This projection involves an α-d relative-motion function, and the falloff of the tail of this function bears the imprint of the $\alpha+d$ separation energy. Since the no-core shell model is intended to be a consistent model for all light nuclei, it is a relevant test to examine whether it reproduces the separation energies. In fact, the separation energy should be calculated from binding energies obtained in fully consistent state spaces, which is not exactly so in Ref. [1]. The state space used for ^{6}Li is restricted by $2\hbar\omega$ more than those of α and d; thus the breakup energy implied by the ^{6}Li wave function may differ from 0.21 MeV. Nevertheless, it looks likely that such a major discrepancy cannot result from such a minor mismatch between the state spaces. This value of the separation energy seems to imply that the model is not realistic enough (i.e., it is still too restrictive).

Since the cluster-model wave function of ^{6}Li contains many configurations belonging to several different separation energies, it would be difficult to demonstrate the strong dependence of the quadrupole moment on them. Just to give an

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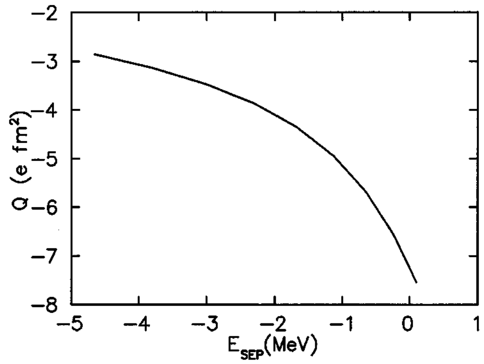

FIG. 1. The quadrupole moment of the ground state of ^{7}Li as a function of its $\alpha+t$ separation energy in an $\alpha+t$ cluster model. The experimental separation energy is 2.47 MeV, and the quadrupole moment is -4.06 e fm^2 [2].

indication of the magnitude of such a dependence, in Fig. 1 we show the quadrupole moment of the ground state of ^{7}Li in an $\alpha+t$ cluster model, using the Minnesota effective nucleon-nucleon force [9]. To mimic the situation in Ref. [1], the exchange mixture parameter of the interaction is varied such that the energy of ^{7}Li changes, while the binding energies of α and t remain fixed. We show Q as a function of the $\alpha+t$ separation energy. One can see that the quadrupole moment is very sensitive to this quantity. The ^{6}Li quadrupole moment is likely to behave in a similar way. If so, then one could easily reproduce the ^{6}Li quadrupole moment in this framework by an unphysical artifice: just choose the parameters so that the energy may exceed the $\alpha+d$ threshold by a suitable amount, and treat the nucleus as if it were still bound. This is exactly how the shell model describes ^{6}Li, and a quadrupole moment produced in this way cannot be regarded as physical.

In summary, a theoretical value for the ^{6}Li quadrupole moment can only be accepted as physically meaningful if the model produces the correct separation energies, especially for the most important $\alpha+d$ partition. Without this, a reproduction of the experimental value can only be fortuitous.

The problem with the low-lying positive-parity states of ^{5}He is even more acute: while the asymptotics of a system of loosely bound fragments can certainly be handled with a square-integrable basis, those of resonant states cannot. If we set the zero point of the energy scale of the A-nucleon system to the total A-body disintegration threshold, then any state below this threshold has a negative energy. This would imply an exponentially damped bound-state A-body asymptotic wave function [10]

$$\Psi_A \sim \exp(-k_A\rho_A) \quad \text{for} \quad \rho_A \to \infty. \tag{1}$$

Here ρ_A is the hyper-radius, $\rho_A^2=\Sigma_i r_i^2$, where $\mathbf{r}_i$ are the one-particle position vectors, and $k_A=(2m_N E_A/\hbar^2)^{1/2}$, where E_A is the binding energy of the A-body system, and m_N is the nucleon mass. Such a Ψ_A can really be expanded in terms of square-integrable functions, as in a shell model. However, the boundary condition (1) only applies if there is no breakup channel below E_A. If there is a two-body ($A=B+C$) breakup channel below E_A, then the correct boundary condition is [11]

$$\Psi_A \sim \exp(-k_A\rho_A)+\Phi^B\Phi^C[x\ \exp(-ikr) + y\ \exp(ikr)] \quad \text{for}\ \rho_A,\ r\to\infty. \tag{2}$$

Here r is the distance between the fragments B and C, the functions Φ are the intrinsic states of B and C with binding energies E_B and E_C, $k=[2\mu(E_A-E_B-E_C)/\hbar^2]^{1/2}$, and μ is the reduced mass in this partition. A scattering "state," of energy E_A, that obeys Eq. (2) will be regarded as a (resonant) *state of the nucleus* if $S=-y/x$ (the "S matrix") has a pole at the complex energy $E_A-i\Gamma/2$, where Γ is the total width.

Square-integrable bases, however large they are, are obviously unable to obey the boundary condition in Eq. (2), so whatever they predict for states above breakup thresholds is to be taken with reservation. This applies to the low-lying positive-parity states of ^{5}He, which are above the $\alpha+n$ threshold. The main component of the $1/2^+$ state, e.g., is $\pi(0s)^2\nu(0s)^2(1s)^1$, which has a large overlap with the $\alpha+n$ continuum. Thus this state would be very strongly coupled to the continuum, which may have a very strong effect.

We have performed a search for such states in a large-space cluster model whose wave function is

$$\Psi=\sum_{S,L}\left(\mathcal{A}\{[(\Phi^\alpha\Phi^n)_S\chi_L^{\alpha n}(\boldsymbol{\rho}_{\alpha n})]_{JM}\} + \mathcal{A}\{[(\Phi^d\Phi^t)_S\chi_L^{dt}(\boldsymbol{\rho}_{dt})]_{JM}\}\right), \tag{3}$$

where $\mathcal{A}$ is the intercluster antisymmetrizer, the cluster intrinsic states Φ are translation invariant $0s$ harmonic oscillator shell-model states for the α particle, deuteron, and triton, the vectors $\boldsymbol{\rho}$ are the intercluster Jacobi coordinates, and $[\cdots]$ denotes angular momentum coupling. In the sum over S and L all possible configurations are included. It is important to note that bound-state-type cluster-model calculations of this type do produce a low-lying $1/2^+$ state [12], just as the shell model does (and, somewhat higher up, $3/2^+$ and $5/2^+$ states as well). Here, however, we impose on the intercluster relative-motion functions χ the correct unbound-state asymptotics. To avoid any ambiguity in the recognition of a resonance in the phase shift $\delta=\frac{1}{2}\arg S$, we searched for complex-energy poles of the S matrix directly. Both an analytic continuation method [13] and the complex scaling method [14] were used. The $3/2^-$ and $1/2^-$ states were found, but the next level was the $3/2^+$ state at 16 MeV excitation energy. No sign of any low-lying $1/2^+$, $3/2^+$, or $5/2^+$ states was found. The inclusion of a few monopole breathing excitations of α did not change the situation either. This rules out even the exotic possibility that the low-lying positive-parity states are Pauli resonances [15], since with the departure from the single oscillator description of the α cluster the configurations that might produce Pauli resonances get automatically included.

To produce a low-energy $1/2^+$ state artificially, we made the intercluster binding stronger, while keeping the cluster binding energies fixed, by changing a mixing parameter of the N-N interaction. Then we let the mixing parameter tend toward its physical value, and followed the position of the $1/2^+$ pole. The pole moved rapidly towards higher energies and, for example, it was found at 19 MeV excitation energy with a width of 34 MeV while the mixing parameter was still highly nonphysical; indeed, the same parameter value produced deeply bound $3/2^-$ and $1/2^-$ states. Further change of the mixing parameter in the direction of its correct value pushed this $1/2^+$ state to even higher energies with larger widths.

All in all, in a model that handles the asymptotics correctly, the low-lying positive-parity states of ^{5}He do not show up. Although the basis used by Zheng *et al.* [1] is probably more flexible than ours to describe the correlated short-range motion of the nucleons, it is very difficult to imagine that an improvement of our model in this direction would bring down high-lying positive-parity states from the upper region of the continuum. On the other hand, with a bound-state treatment, it is straightforward to lower any high-energy resonant state close to the lowest-lying threshold. Indeed, when an oscillator basis is enlarged, the pseudobound states will converge to this threshold, and not to the correct resonance energy, even if there exists a resonance [16]. Nevertheless, it is still to be proven whether or not the nonphysical boundary condition results in the appearance of these states in the calculations of Zheng *et al.* The direct way to check this would be to supplement the wave function of Ref. [1] by an $\alpha+n$ cluster term which describes the correct asymptotics. This could be done, for example, in a cluster-configuration shell model [17]. An indirect indication as to whether these states are real or spurious could be obtained more simply by examining the stability of their energies against changes in the size of the square-integrable basis. Resonant states produced by a square-integrable basis are distinguishable from spurious states (i.e., bound-state approximants to plain continuum states) by their energies being stable against enlargements of the basis *within some interval of basis sizes*. The resonance energies are then given by the energies corresponding to the centers of these intervals [16].

Just to give an example that the incorrect boundary condition can incur spurious states, here we show the case of ^{8}Li. This nucleus is described in a three-cluster $\alpha+t+n$ model with the basis containing a number of different angular momenta [18]. Expanding all intercluster relative-motion functions in terms of square-integrable functions, one gets, from the diagonalization of the Hamiltonian, two 2^+ states below the $\alpha+t+n$ threshold, at binding energies 4.2 MeV and 1.1 MeV (relative to the three-cluster threshold), respectively. Experiment has only produced one 2^+ state in this region, the ground state. The square-integrable basis is seemingly adequate, because we are below the three-cluster threshold. However, the 1.1 MeV energy state is above the ^{7}Li$+n$ two-body breakup threshold, which means that the correct boundary condition has to contain a ^{7}Li$+n$ scattering term. Supplementing our wave function by such a term, the 1.1 MeV 2^+ state disappears immediately, showing that this state was an artifact brought about by the incorrect boundary condition.

By this analogy, we suggest that the low-lying positive-parity states of ^{5}He could also disappear if the proper boundary condition were taken into account. Be that as it may, we cannot claim that this would disprove the existence of the states in question. But certainly, before further efforts are spent on understanding the nature of these states, the empirical evidence for their existence should be reconsidered.

In conclusion, the reproduction of the negative quadrupole moment of ^{6}Li and the low-lying positive-parity states of ^{5}He by Zheng *et al.* [1] in a shell model cannot be regarded as well founded because the aspects of few-body dynamics underlying these effects are treated improperly in that model. We think that the no-core shell model has been a significant advance towards understanding nuclear structure, and it is all the more important to understand its limitations as well.

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[1] D. C. Zheng, J. P. Vary, and B. R. Barrett, Phys. Rev. C **50**, 2841 (1994).
[2] F. Ajzenberg-Selove, Nucl. Phys. **A490**, 1 (1988).
[3] V. I. Kukulin, V. N. Pomerantsev, Kh. D. Razikov, V. T. Voronchev, and G. G. Ryzhikh, Nucl. Phys. **A586**, 151 (1995).
[4] B. V. Danilin, M. V. Zhukov, A. A. Korsheninnikov, and L. V. Chulkov, Yad. Fiz. **53**, 71 (1991) [Sov. J. Nucl. Phys. **53**, 45 (1991)].
[5] N. W. Schellingerhout, L. P. Kok, S. A. Coon, and R. M. Adam, Phys. Rev. C **48**, 2714 (1993).
[6] A. Csótó and R. G. Lovas, Phys. Rev. C **46**, 576 (1992).
[7] M. Unkelbach and H. M. Hofmann, Few-Body Syst. **11**, 143 (1991).
[8] S. Weber, M. Kachelriess, M. Unkelbach, and H. M. Hofmann, Phys. Rev. C **50**, 1492 (1994).
[9] D. R. Thompson, M. LeMere, and Y. C. Tang, Nucl. Phys. **A286**, 53 (1977); I. Reichstein and Y. C. Tang, *ibid.* **A158**, 529 (1970).
[10] L. M. Delves, Nucl. Phys. **20**, 275 (1960).
[11] S. P. Merkur'ev, Yad. Fiz. **19**, 447 (1974) [Sov. J. Nucl. Phys. **19**, 222 (1974)].
[12] R. G. Lovas, A. T. Kruppa, and J. B. J. M. Lanen, Nucl. Phys. **A516**, 325 (1990).
[13] A. Csótó, R. G. Lovas, and A. T. Kruppa, Phys. Rev. Lett. **70**, 1389 (1993).
[14] A. T. Kruppa, R. G. Lovas, and B. Gyarmati, Phys. Rev. C **37**, 383 (1988); A. Csótó, *ibid.* **49**, 3035 (1994).
[15] S. Saito, Prog. Theor. Phys. Suppl. **62**, 11 (1977).
[16] R. G. Lovas and M. A. Nagarajan, J. Phys. A **15**, 2383 (1982).
[17] K. Varga, R. G. Lovas, and R. J. Liotta, Nucl. Phys. **A550**, 421 (1992).
[18] A. Csótó, Phys. Lett. B **315**, 24 (1993).