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Microscopic multicluster model of ^{9,10,11}Li

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A microscopic cluster model assuming α-, triton, and single-neutron clusters is applied to the halo nucleus ^{11}Li and to its subsystems ^{9}Li and ^{10}Li. This model is consistent with an earlier successful description of ^{7,8,9}Li. The results for the energies, radii, and other properties of ^{11}Li are satisfactory. The binding of ^{11}Li receives comparable contributions from *p*- and *s*-wave single-particle states. The two-neutron halo of ^{11}Li is confirmed to be prominent although it is reduced by core distortion.

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The most famous halo nucleus is ^{11}Li. Its halo structure is indicated by the prominent interaction cross sections of its collisions [1], by the narrow momentum distribution of its ^{9}Li fragment [2], by the Borromean (i.e., three-particle) nature of the binding between its $^{9}\mathrm{Li}+n+n$ constituents and by its very small two-neutron separation energy.

In ^{9}Li the $0p_{3/2}$ subshell is filled, while in ^{11}Li itself the full $0p$ neutron shell should be closed. It may well be, however, that the sequence of the $0p$ and $1s$ levels is reversed. The nucleus ^{10}Li is not bound, but the sequence of its near-threshold states is expected to determine the nature of the binding of ^{11}Li [3]. The ^{9}Li core may not be passive, and the core distortion (i.e., excitation) must imply complicated Pauli and other correlation effects.

Nevertheless, the theoretical approaches to the description of ^{11}Li are mostly macroscopic or semimicroscopic and are based on the $^{9}\mathrm{Li}+n+n$ three-body picture [4–6]. The occupancy of the core is generally taken into account by an orthogonality condition on the halo neutrons. The models are devised either to reproduce (i) the binding of ^{11}Li by using two-body forces appropriate for the subsystems, $^{10}\mathrm{Li}+n$ and $n+n$, (ii) or the known properties of ^{11}Li by adjusting the interactions phenomenologically.

The binding-energy problem (i) can as yet be solved only roughly because of the uncertainties of our knowledge on ^{10}Li. A 1^+ state and a 2^+ state can be produced in the range where experiments seem to find resonance states, but a disagreement in the widths points to the role of core excitations [7,8]. Microscopic calculations confirm this indication [9]. With the same $^{9}\mathrm{Li}-n$ interaction, ^{11}Li has been found to be underbound by about 1 MeV [6]. This tallies with the case of ^{6}He, and, similarly, must be due to the excitation of the core [10].

Independently of the binding-energy problem, the gross properties of ^{11}Li can be reproduced by three-body models whose parameters are adjusted to yield the correct energy, ε, with respect to the $^{9}\mathrm{Li}+n+n$ threshold [problem (ii)]. Three-body calculations predict that the halo is indeed much more extensive than the core [6].

Problem (ii) has also been solved in a microscopic $^{9}\mathrm{Li}+n+n$ model with simple central interactions [11]. In this model all core distortions that go with *p*-shell excitations are taken into account, at the expense of grossly restricting the relative-motion configurations. The nucleus ^{11}Li is described pretty well, but the corresponding $^{9}\mathrm{Li}+n$ model yields a bound ^{10}Li, which shows that the binding-energy problem has not been solved.

In the present work the energies of ^{10,11}Li and the other properties of ^{11}Li have been reproduced *simultaneously*. This has been achieved in a fully microscopic $\alpha+t+n+\ldots+n$ cluster model, an extension of that applied to ^{7,8,9}Li earlier [12]. The approach is unique in that the core distortion is taken into account very carefully; this is a fully dynamical correlated six-cluster model for ^{11}Li, in which all symmetries are observed exactly. This is feasible owing to the correlated Gaussian bases used [13].

The starting point is the description of ^{9}Li. In the $\alpha+t+n+n$ model [12] its wave function can be written as $\Psi^{JM}_{^{9}\mathrm{Li}}=\Sigma_i C_i \psi_i^{JM}(^{9}\mathrm{Li})$, with

$$\psi_i^{JM}(^{9}\mathrm{Li})=\mathcal{A}\{[\Phi_S(^{9}\mathrm{Li})\mathrm{e}^{-(1/2)\tilde{\boldsymbol{\rho}}A_i\boldsymbol{\rho}}\theta_{l^i_1 l^i_2 l^i_3 L}]_{JM}\},$$

$$\Phi_{SM_S}(^{9}\mathrm{Li})=\Phi_\alpha(\xi_{1234})[\Phi_{t(1/2)}(\xi_{567})[\chi_{(1/2)}(8)\times\chi_{(1/2)}(9)]_{s^i_{12}}]_{SM_S},$$

where $\mathcal{A}$ is an antisymmetrizer, Φ_j $(j=\alpha,t)$ are cluster intrinsic states, $\chi_{(1/2)m_s}$ are spin states (the isospin states are suppressed), $\mathrm{e}^{-(1/2)\tilde{\boldsymbol{\rho}}A_i\boldsymbol{\rho}}\theta_{l^i_1 l^i_2 l^i_3 L M_L}$ is a correlated Gaussian function of the Jacobi coordinates $\{\boldsymbol{\rho}_1,\boldsymbol{\rho}_2,\boldsymbol{\rho}_3\}$ describing the four-cluster relative motion, and the square bracket denotes angular-momentum coupling. The expression $\tilde{\boldsymbol{\rho}}A_i\boldsymbol{\rho}$ is chosen

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so that $e^{-(1/2)\tilde{\boldsymbol{\rho}}A_i\boldsymbol{\rho}}$ may reduce to a product of Gaussians of independent intercluster relative coordinates $\{\boldsymbol{\rho}'_1,\boldsymbol{\rho}'_2,\boldsymbol{\rho}'_3\}$. The factors $\theta_{l_1^i l_2^i l_3^i LM_L}$ are coupled products of the solid spherical harmonics of $\boldsymbol{\rho}'_1,\boldsymbol{\rho}'_2,\boldsymbol{\rho}'_3$. The summation over i produces all sets $\{\boldsymbol{\rho}'_1,\boldsymbol{\rho}'_2,\boldsymbol{\rho}'_3\}$ and runs over all angular momenta of any significance. (For details, see Ref. [12].) Only the dominant configurations with $(SL)J=(\frac{1}{2}1)\frac{3}{2}$ have been kept.

The Minnesota nucleon-nucleon force [14] was used, with spin-orbit and Coulomb terms, just as in Ref. [12]. The basis was constructed stepwise by stochastic optimization [13]. A smaller and yet satisfactory basis (with dimension 50) was obtained by optimizing A_i more extensively. (A compact basis helps to keep the corresponding ^{11}Li calculation manageable.) To improve the $\alpha+t+n+n$ energy ε, the mixing parameter u [14] was changed from 1.0 to 1.0285. The result, $|\varepsilon|=5.91$ MeV, is close to the experimental value, 6.09 MeV. This u sets ^{10}Li unbound.

We then describe ^{10}Li as a ^{9}Li-like structure, generated by the basis of ^{9}Li, coupled with a neutron in a relative s or p state: $\Psi^{JM}_{^{10}\mathrm{Li}}=\Sigma_{ij}C'_{ij}\psi^{JM}_{ij}(^{10}\mathrm{Li})$, with

$$\psi^{JM}_{ij}(^{10}\mathrm{Li})=\mathcal{A}\{[[\psi^{J_9}_i(^9\mathrm{Li})\chi_{(1/2)}(10)]_{S_i}\psi^{(\beta_j)}_{0l}(\boldsymbol{\rho}_4)]_{JM}\},$$

where $\boldsymbol{\rho}_4$ is the ^{9}Li$-n$ relative-distance vector. The single neutron is described by a combination of nodeless harmonic-oscillator states $\psi^{(\beta)}_{0lm}(\boldsymbol{r})\propto r^l e^{-(1/2)\beta r^2}Y_{lm}(\hat{\boldsymbol{r}})$. Each core state is accompanied by eight such functions, chosen by stochastic sampling, the dimension totaling 400.

The coefficients C'_{ij} are determined by diagonalization of the Hamiltonian. This is thus a sophisticated cluster-distortion model, in which a large subspace of the ^{9}Li intrinsic motion is taken into account: that which carries the angular-momentum quantum numbers of the g.s.

The system was enclosed in a box by prescribing $(\beta_j)^{-1/2}\leqslant 6$ fm. Square-integrable bases can only produce real-energy discrete states. The states that are stable against changes in the ''box size'' correspond to resonances, the others are to be considered discretized continuum states. It is very probable that the energy of the lowest-lying resonance state (if a resonance exists) in each quantum-number set agrees roughly with what could be obtained by imposing the proper outgoing-wave boundary condition. Indeed, the energies only slightly change in a larger box $[(\beta_j)^{-1/2}\leqslant 10$ fm]. If, in a particular partial wave, the lowest-lying state is a virtual state, it is likely that the low-lying positive-energy discrete states will overlap with the true virtual state substantially.

The level sequence obtained is as follows (the energy ε with respect to the ^{9}Li$+n$ threshold in parentheses): 1^+ (0.39 MeV), 2^+ (0.55 MeV), 2^- (1.56 MeV), 1^- (1.74 MeV), 0^+ (2.12 MeV). When the box is made larger, the two lowest levels slip slightly closer to the threshold (the 1^+ state is at 0.31 MeV), but the energy difference between them remains the same. The positive-parity states come from the p orbits, and can be assumed to correspond to the experimentally observed levels [15]. To find a low-lying 0^+ state is surprising since in the shell model it would imply a high-lying $1p_{3/2}$ orbit as the $0p_{3/2}$ orbits are filled. In a cluster model, however, none of the shell-model orbits is fully occupied [16]. The low-lying 0^+ state confirms that the core excitation is significant.

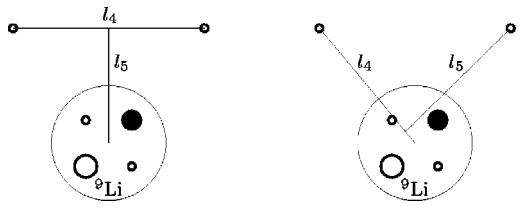

FIG. 1. T- and Y-type Jacobi coordinates for ^{9}Li$+n+n$, with the angular momenta belonging to $\boldsymbol{\rho}_4,\boldsymbol{\rho}_5$ shown. Notation: α: ●; triton: ○; neutron: ◦. For $\alpha+t+n+n$ all relative vectors and l_1, l_2, l_3 values given in Ref. [12] are included.

The g.s. (1^+) and the first excited state (2^+) are resonance states, but one cannot draw definite conclusion for the other states $(1^-,2^-)$ from the present calculation. They obviously have large s-wave components in the ^{9}Li$-n$ relative motion. In a purely attractive local potential a near-threshold unbound s state is mostly a virtual state $[E\equiv(\hbar^2/2m)k^2<0,\ k=-i\gamma$, with real $\gamma>0]$ or an unphysical resonance $(E=E_R+iE_I$, with $E_R,E_I<0$, and $k=\kappa-i\gamma$, with $\kappa,\gamma>0$, $\kappa<\gamma)$, and a few-body system may behave similarly.

The wave function of ^{11}Li is constructed by adding two neutrons to ^{9}Li. The ^{9}Li$+n+n$ picture is related to the underlying $\alpha+t+n+n+n+n$ model (see Fig. 1) through the wave function $\Psi^{JM}_{^{11}\mathrm{Li}}=\Sigma_{ij}C''_{ij}\psi^{JM}_{ij}(^{11}\mathrm{Li})$, with

$$\psi^{JM}_{ij}(^{11}\mathrm{Li})=\mathcal{A}\{[\psi^{J_9}_i(^9\mathrm{Li})[e^{-(1/2)\tilde{\boldsymbol{\rho}}'A'_j\boldsymbol{\rho}'}\theta'_{l^j_4 l^j_5 l^j_{45}}\chi_{sj}]_{Jj}]_{JM}\},$$

where $\boldsymbol{\rho}'=\{\boldsymbol{\rho}_4,\boldsymbol{\rho}_5\}$ are ^{9}Li$+n+n$ Jacobi coordinates, the 2×2 matrix A'_j is allowed to take on values representing both Y- and T-type arrangements, and χ_s is the combined spin function of the two extra neutrons: $\chi_s=[\chi_{1/2}(10)\chi_{1/2}(11)]_s$. Each intermediate angular momentum is restricted to values of 0 or 1. The two-neutron states are then coupled to the $\frac{3}{2}^-$ state of ^{9}Li to form the g.s. of ^{11}Li with $J^\pi=\frac{3}{2}^-$.

The basis for ^{11}Li has been set up by combining stochastic and direct techniques. First 20 basis states were constructed in each configuration by stochastic optimization. A configuration is defined by the ^{9}Li$+n+n$ Jacobi coordinates (T or Y, see Fig. 1) and by the set of quantum numbers given in Table I. This basis is not extensive enough to produce binding. Then each relative-motion function was expanded in terms of three Gaussians, whose widths form geometrical progressions, with optimized parameters. The 50 functions for the core, with eight ^{9}Li$+n+n$ configurations and 3×3 relative-motion Gaussians in each configuration total 3600 basis states. These were added to the stochastically chosen elements. This model space seems to be sufficiently large, at least, as far as the ^{9}Li$+n+n$ relative motion is concerned. So the solution must be reasonably accurate.

TABLE I. The energy (in MeV), with respect to the ^{9}Li$+n+n$ threshold, and proton, neutron, and matter rms radii (in fm) of ^{11}Li as produced individually by each configuration in the full and in a frozen-core correlated Gaussian model.

Configuration					Full model				Frozen model			
	l_4	l_5	l_{45}	s	ε	r_p	r_n	r_m	ε	r_p	r_n	r_m
T	0	0	0	0	−0.22	2.44	3.15	3.12	−0.05	2.13	3.14	3.12
T	1	1	0	0	−0.04	2.36	3.07	3.04	0.24	2.16	3.29	3.23
T	1	1	1	1	0.15	2.47	3.41	3.35	0.52	2.16	3.27	3.23
Y	0	0	0	0	0.13	2.47	3.40	3.34	0.61	2.17	3.24	3.19
Y	0	0	0	1	−0.25	2.42	3.11	3.11	−0.09	2.14	3.17	3.16
Y	1	1	0	1	−0.19	2.41	3.02	2.98	−0.11	2.13	3.13	3.10
Y	1	1	1	1	−0.15	2.40	3.01	2.98	−0.07	2.13	3.14	3.11
Y	1	1	1	0	−0.11	2.39	2.97	2.95	0.35	2.15	3.31	3.25
all					−0.34	2.43	3.09	3.03	−0.12	2.15	3.21	3.15

With $u=1.0285$, the g.s. of ^{11}Li is at $\varepsilon=-0.34$ MeV below the ^{9}Li$+n+n$ threshold, which agrees with the experimental value, $\varepsilon=-0.25\sim-0.40$ MeV [17,18]. Thus, at least at the low-precision level of the experimental ^{10}Li energy, the binding-energy problem appears to be solved. Moreover, considering the models of ^{7,8,9}Li [12], one can say that all Li isotopes with $7\leqslant A\leqslant 11$ are described consistently by the microscopic multicluster model. (Remember that the readjustment of u is needed just to mock up the truncation of the core g.s.)

Table I shows the configurations included, the energies and the point-matter root mean square (rms) radii produced by the individual configurations and by all. The important configurations produce almost the same energy, whether they involve T or Y arrangements, $l_4=l_5=0$ or 1. It is thus fair to say that s, p, and, possibly, higher-l orbits appreciably contribute to the binding. Note, however, that these configurations are highly nonorthogonal. The Y-like arrangement is close to the shell-model picture, and the T-type configurations, if expressed in Y terms, involve many, in principle infinitely many, orbits. (The coordinates used in the shell model form a V-pattern pointed at the core. The Y-type Jacobi coordinates are very close to these.) The calculation was repeated by freezing the ^{9}Li core to its g.s. (i.e., by neglecting its distortion). The table shows that in the frozen approximation 100-500 keV is lost of the ^{9}Li$+n+n$ energy, which is quite substantial for a halo nucleus.

To shed new light on the binding mechanism, we calculated the overlap of the wave function with Y-like states that imitate shell-model configurations of various l,s and produce rms radii of $\sim$3 fm. Since the Y-pattern differs from the V-pattern of the shell model, these states are slightly nonorthogonal; nevertheless, the squared overlaps in Table II do add up approximately to unity. The results show that the p orbits are important but so are the s and d orbits. There may be appreciable overlaps with configurations containing even higher-l orbits.

The properties of ^{9,11}Li are compared with experiment in Table III. The ^{9}Li model truncated to provide the starting point for ^{11}Li gives basically the same values as the original

TABLE II. Overlap of the ^{11}Li wave function with various Y-type configurations imitating shell-model configurations.

Arrangement	l_4	l_5	l_{45}	s	Overlap
Y	0	0	0	0	0.24
Y	0	0	0	1	0.42
Y	1	1	0	0	0.32
Y	1	1	0	1	0.37
Y	1	1	1	0	0.28
Y	1	1	1	1	0.49
Y	2	2	0	0	0.12
Y	2	2	0	1	0.21
Y	2	2	1	0	0.14
Y	2	2	1	1	0.23
Y	2	2	2	1	0.17

(''full'') model [12], except for the quadrupole moment (Q), whose agreement with experiment has been broken by the truncation. (Note that $u=1$ in the full model of ^{9}Li and $u=1.0285$ elsewhere.) The rms radii of ^{11}Li calculated in the full model agree with the data of Ref. [19] fairly well. The matter radius is close to the other experimental estimate [1] as well. The proton radius of the frozen ^{11}Li is larger than that of ^{9}Li because the core center of mass in ^{11}Li fluctuates with respect to the nuclear one; a further substantial increase in the full model is due to core distortion. The difference between ^{9}Li and ^{11}Li in the neutron radii reflects the pronounced neutron halo; the difference between the frozen and the full models of ^{11}Li is a trivial binding-energy effect.

It would be interesting to see what the model predicts for the halo radius r_h itself. To avoid the fairly involved calculations required, one can resort to an approximate picture. In the no-distortion limit, the core radii may be identified with the radii of ^{9}Li. Furthermore, with the Pauli and c.m. effects

TABLE III. Properties of ^{9}Li in the full and truncated (tr.) models and of ^{11}Li in the full and frozen (fr.) models. The energies are measured from the two-neutron thresholds. The experimental (exp.) cross sections (see text) and radii are from Ref. [1] and the electromagnetic moments from Ref. [20].

A		ε (MeV)	r_p (fm)	r_n (fm)	r_m (fm)	Q (e fm^2)	μ (μ_N)	$\sigma_{\rm reac}$ (mb)
9	full [a]	−8.05	2.10	2.52	2.39	−2.74	3.43	
	tr.	−5.91	2.12	2.54	2.41	−3.37	3.40	799±3
	exp.	−6.09	2.18	2.39	2.32	−2.74	3.44	796±6
11	fr.	−0.12	2.15	3.21	3.15	−3.52	3.21	1054±2
	full	−0.34	2.43	3.09	3.03	−3.71	3.23	1023±2
		−0.340 [b]	2.88 [d]	3.21 [d]	3.12 [d]			
	exp.	−0.295 [c]	2.24 [e]	3.26 [e]	3.01 [e]	3.12 [f]	3.67	1056±14

[a]Reference [12].
[b]Reference [17]; error: ±0.05.
[c]Reference [18]; error: ±0.035.
[d]Reference [1].
[e]Reference [19].
[f]$|Q|$.

disregarded, $r_m^2(^{11}\mathrm{Li}) \approx \frac{1}{11}[9r_m^2(^9\mathrm{Li}) + 2r_h^2(^{11}\mathrm{Li})]$ and $r_n^2(^{11}\mathrm{Li}) \approx \frac{1}{8}[6r_n^2(^9\mathrm{Li}) + 2r_h^2(^{11}\mathrm{Li})]$. These formulas yield, respectively, $r_h = 4.98$ and 4.375 fm with the full model and 5.37 and 4.71 fm with the frozen model. All these numbers are close to what is produced by an analysis (5.1 fm [23]) and a theoretical value (4.72 fm [24]), and their scatter reflects the error in the model assumptions.

The calculated ^{11}Li quadrupole moment differs from experiment just as in the truncated ^{9}Li model; the discrepancy can thus be attributed to the core truncation. (The experimental value for ^{11}Li is assumed to be negative.) The reaction cross sections σ_{reac} of the collisions of ^{9,11}Li with ^{12}C at 800 MeV per nucleon have been calculated in the Glauber model with the multiple nucleon-nucleon collisions taken into account to all orders. The details of this calculation will be given elsewhere [21]. These cross sections can hardly differ from the interaction cross sections since ^{11}Li has no particle-bound excited state [22], and the experimental data quoted are actually interaction cross sections. The theory is in good accord with experiment. This reaction model is very reliable, thus the simultaneous agreement in σ_{reac} and r_m between the empirical and theoretical values implies that the empirical r_m value must also be reliable.

One can sum up the results of this work as follows.

The energies of ^{10}Li and ^{11}Li and the properties of ^{11}Li have been reproduced simultaneously without extra adjustments. With this, the binding energy problem has been solved, and a comparison with previous work [11] indicates that this degree of sophistication is in fact necessary. The model is almost fully consistent for the nuclear chain $^{7-11}$Li.

The results give some insight into the binding mechanism of these nuclei. The g.s. of ^{10}Li is of *p*-wave nature. The existence of a near-threshold *s*-wave virtual state is not excluded, but it makes no sense to regard it as the g.s. The binding of ^{11}Li receives approximately equal contributions from *p*- and *s*-wave single-particle states.

Core distortion effects appear to be significant, which limits the validity of the three-body models and emphasizes the need for the multicluster approach. The distortion dilates the core, which makes the neutron skin thinner, but does not invalidate the two-neutron halo picture.

All in all, this is the most sophisticated model hitherto applied to the paradigmatic halo nucleus ^{11}Li, and it is the first one to appear to be fully satisfactory.

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