

Explicitly correlated wave function for a boron atom

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We present results of high-precision calculations for a boron atom's properties using wave functions expanded in the explicitly correlated Gaussian basis. We demonstrate that the well-optimized 8192 basis functions enable a determination of energy levels, ionization potential, and fine and hyperfine splittings in atomic transitions with nearly parts per million precision. The results open a window to a spectroscopic determination of nuclear properties of boron including the charge radius of the proton halo in the ^{10}B nucleus.

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INTRODUCTION

While for hydrogenic ions the nonrelativistic wave function is known exactly, for all larger atomic systems it has to be obtained numerically, most often with the help of the variational principle. The numerical precision achieved for a few electron systems can, nevertheless, be very high. For example, nonrelativistic energies of the He atom are known with more than 20 digits of accuracy [1–3], of Li with 15 digits [4, 5], and very recently the precision achieved for the Be atom reached 11 significant digits [6–8]. The computational approach employed in all those atomic studies is based on explicitly correlated functions of the exponential or Gaussian form, which are the best known representations of the nonrelativistic wave function. For three-electron systems, the most accurate solution of the Schrödinger equation is obtained with the Hylleraas (exponential times polynomial) basis functions [4, 5, 9]. In such systems, the accuracy of the theoretical predictions for transition energies and isotope shifts is limited by the approximate treatment of higher-order $\sim m\alpha^{6,7}$ QED corrections rather than by numerical inaccuracies of the nonrelativistic wave function. Methods with Hylleraas functions have been extended to four-electron atomic systems but only for some restricted selection of basis functions, because of significant difficulties in evaluation of matrix elements [10, 11]. Even more difficult integrals appear in the matrix elements of relativistic operators. Unquestionably, significant efforts have to be made to improve the Hylleraas approach, in order for it to be practical for the four and more electron systems. Therefore, at present, the method of choice for such systems is that based on explicitly correlated Gaussian (ECG) functions. The effectiveness of the ECG functions in treating few-electron problems has already been demonstrated by high-precision calculations of the nonrelativistic energies of atomic and molecular systems [12–17]. In particular, for the beryllium atom the highest accuracy has been obtained using the ECG functions [7, 18–21]. The main advantage of the ECG method is that the underlying integration is manageable and very fast in numerical evaluation due to the compact formulas involving only elementary functions. On the other hand, the Gaussian functions have the drawback of improper

asymptotic behavior since they decay too fast at long inter-particle distances. They also have an incorrect short-range form and fail to correctly describe the Kato cusp. However, these two flaws can be overcome if one employs a sufficiently large and well-optimized ECG basis set. The issue is subtler in calculations of relativistic and QED properties, in which the local inaccuracies of the wave functions result in significant numerical loss of mean values. One has to carefully optimize over a large number (oftentimes exceeding 10^5) of variational parameters matching local behavior of the exact wave function and employ dedicated techniques which accelerate the convergence of nearly singular matrix elements [22]. An additional drawback of the approach based on fully correlated functions is the cost resulting from antisymmetrization of the wave function which grows like $N!$ with the number of electrons N .

In this paper we demonstrate that in spite of this high evaluation costs, the methods based on ECG functions may give a spectroscopic accuracy for five-electron systems, such as the boron atom, in a realistic computational time. We report on the calculation of nonrelativistic energies of the ground 2^2P and the excited 3^2S levels, and the leading relativistic corrections including the fine and hyperfine structure of the ground state. The achieved numerical accuracy is several orders higher than those of any previous calculations and not always in agreement with them. In addition, we provide accurate results for a four-electron B^+ ion needed to determine the ionization potential of the boron ground state.

NONRELATIVISTIC HAMILTONIAN AND CORRECTIONS

The determination of accurate wave functions corresponding to the nonrelativistic, clamped nucleus Hamiltonian (in natural units)

$$H_0 = \sum_a \frac{p_a^2}{2m} - \sum_a \frac{Z\alpha}{r_a} + \sum_{a>b} \frac{\alpha}{r_{ab}}. \quad (1)$$

is the main subject of this paper. If the wave function Φ is determined, all the corrections to the energy E_0 in the following perturbative expansion in the fine-structure constant

$\alpha \sim 1/137$

$$E = E^{(2)} + E^{(4)} + E^{(5)} + E^{(6)} + \dots, \quad E^{(n)} \sim m\alpha^n \quad (2)$$

can be expressed in terms of expectation values $\langle \Phi | \dots | \Phi \rangle \equiv \langle \dots \rangle$ of known operators. Complete nonrelativistic energy $E^{(2)}$ consists of the clamped nucleus energy E_0 and the kinetic energy of the nucleus H_N , which can be calculated in the center of mass frame as a small perturbation,

$$H_N = \frac{p_N^2}{2m_N} = \frac{m}{m_N} \left(\sum_a \frac{p_a^2}{2m} + \sum_{a<b} \frac{\vec{p}_a \cdot \vec{p}_b}{m} \right), \quad (3)$$

where m_N is the nuclear mass. The leading relativistic $E^{(4)}$ correction is calculated as the mean value of the Breit-Pauli Hamiltonian given by

$$H^{(4)} = H_{\text{ns}} + H_{\text{fs}} + H_{\text{hfs}}, \quad (4)$$

$$H_{\text{ns}} \equiv \sum_a \left[-\frac{p_a^4}{8m^3} + \frac{Z\alpha\pi}{2m^2} \delta^3(r_a) \right] \quad (5)$$

$$+ \sum_{a>b} \left[\frac{\pi\alpha}{m^2} \delta^3(r_{ab}) - \frac{\alpha}{2m^2} p_a^i \left(\frac{\delta^{ij}}{r_{ab}} + \frac{r_{ab}^i r_{ab}^j}{r_{ab}^3} \right) p_b^j \right],$$

$$H_{\text{fs}} \equiv \sum_a \frac{Z\alpha}{4m^2 r_a^3} \left[(g-1) \vec{r}_a \times \vec{p}_a \right] \cdot \vec{\sigma}_a$$

$$+ \sum_{a \neq b} \frac{\alpha}{4m^2 r_{ab}^3} \vec{\sigma}_a \cdot \left[g \vec{r}_{ab} \times \vec{p}_b - (g-1) \vec{r}_{ab} \times \vec{p}_a \right]$$

$$+ \sum_{a>b} \frac{\alpha g^2}{16m^2 r_{ab}^3} \sigma_a^i \sigma_b^j \left(\delta^{ij} - \frac{3r_{ab}^i r_{ab}^j}{r_{ab}^2} \right). \quad (6)$$

The leading order Hamiltonian for the hyperfine splitting is

$$H_{\text{hfs}} \equiv \sum_a \left[\frac{1}{3} \frac{Z\alpha g g_N}{m m_N} \vec{\sigma}_a \cdot \vec{I} \pi \delta^3(r_a) \right. \\ \left. + \frac{Z\alpha g_N}{2m m_N} \vec{I} \cdot \frac{\vec{r}_a}{r_a^3} \times \vec{p}_a \right. \\ \left. - \frac{Z\alpha g g_N}{8m m_N} \frac{\sigma_a^i I^j}{r_a^3} \left(\delta^{ij} - 3 \frac{r_a^i r_a^j}{r_a^2} \right) \right. \\ \left. + \frac{Q_N}{6} \frac{\alpha}{r_a^3} \left(\delta^{ij} - 3 \frac{r_a^i r_a^j}{r_a^2} \right) \frac{3 I^i I^j}{I(2I-1)} \right], \quad (7)$$

where \vec{I} is the nuclear spin, g is the electron g factor, Q_N is the electric quadrupole moment of the nucleus, and g_N is the nuclear g factor

$$g_N = \frac{m_N}{Z m_p} \frac{\mu}{\mu_N} \frac{1}{I}. \quad (8)$$

It is convenient to rewrite the expectation value of the hyperfine splitting H_{hfs} Hamiltonian in terms of commonly used A_J and B_J coefficients,

$$\langle H_{\text{hfs}} \rangle_J = A_J \vec{I} \cdot \vec{J} + \frac{B_J}{6} \frac{3(I^i I^j)^{(2)}}{I(2I-1)} \frac{3(J^i J^j)^{(2)}}{J(2J-1)}, \quad (9)$$

where \vec{J} is the total electronic angular momentum. For this purpose we decompose H_{hfs}

$$H_{\text{hfs}} = \vec{I} \cdot \vec{G} + \frac{G^{ij}}{6} \frac{3(I^i I^j)^{(2)}}{I(2I-1)}, \quad (10)$$

and these coefficients are

$$A_J = \frac{1}{J(J+1)} \langle \vec{J} \cdot \vec{G} \rangle, \quad (11)$$

$$B_J = \frac{2}{(2J+3)(J+1)} \langle J^i J^j G^{ij} \rangle_J. \quad (12)$$

Higher-order corrections to the atomic energy originate from QED. They are significantly smaller than $E^{(4)}$ because of the higher powers of α :

$$E^{(5)} = \frac{4Z\alpha^2}{3m^2} \left[\frac{19}{30} + \ln(\alpha^{-2}) - \ln k_0 \right] \sum_a \langle \delta^3(r_a) \rangle$$

$$+ \frac{\alpha^2}{m^2} \left[\frac{164}{15} + \frac{14}{3} \ln \alpha \right] \sum_{a<b} \langle \delta^3(r_{ab}) \rangle \quad (13)$$

$$- \frac{7}{6\pi} m \alpha^5 \sum_{a<b} \left\langle P \left(\frac{1}{m\alpha r_{ab}^3} \right) \right\rangle,$$

$$E^{(6)} \approx \frac{\pi Z^2 \alpha^3}{m^2} \left[\frac{427}{96} - 2 \ln(2) \right] \sum_a \langle \delta^3(r_a) \rangle. \quad (14)$$

REDUCTION OF MATRIX ELEMENTS

We represent the wave function Φ^i of the five-electron 2P atomic state in the form

$$\Phi^i = \frac{1}{\sqrt{5!}} \mathcal{A} \left[\sum_n t_n \phi_n^i(\{\vec{r}_a\}) \chi_{\{a\}} \right] \quad (15)$$

where t_n is a linear coefficient, $\chi_{\{a\}}$ is the spin wave function

$$\chi_{\{a\}} = (\alpha_1 \beta_2 - \beta_1 \alpha_2) (\alpha_3 \beta_4 - \beta_4 \alpha_3) \alpha_5 \quad (16)$$

and $\{a\}$ and $\{\vec{r}_a\}$ denote the sequences 1, 2, 3, 4, 5 and $\vec{r}_1, \vec{r}_2, \vec{r}_3, \vec{r}_4, \vec{r}_5$, respectively. The symbol \mathcal{A} denotes antisymmetrization and $\phi^i(\{\vec{r}_a\})$ is a spatial function with Cartesian index i that comes from one of the electron coordinates

$$\phi^i(\{\vec{r}_k\}) = r_m^i \exp \left[- \sum_{k=1}^N a_k r_k^2 - \sum_{l>k=1}^N b_{kl} r_{kl}^2 \right]. \quad (17)$$

The normalization we assume is

$$\sum_i \langle \Phi^i | \Phi^i \rangle = \sum_n \sum_m t_n^* t_m \sum_i \langle \phi_n^i | \phi_m^i \rangle_S = 1 \quad (18)$$

where

$$\langle \phi'^i | \phi^i \rangle_S = \langle \phi'^i(\{\vec{r}_b\}) | \mathcal{P}_{\{a\}} [c_{\{a\}} \phi^i(\{\vec{r}_a\})] \rangle \quad (19)$$

and where $\mathcal{P}_{\{a\}}$ denotes the sum over all permutations of $\{a\}$. From now on we will assume that a repeated Cartesian index

is implicitly summed up. We introduce also another type of a matrix element, which will be used later

$$\langle \phi'^i | Q | \phi^k \rangle_F = \sum_c \langle \phi'^i(\{\vec{r}_a\}) | Q_c \mathcal{P}_{\{b\}} [c_{\{b\}}^{Fc} \phi^k(\{\vec{r}_b\})] \rangle. \quad (20)$$

The c coefficients are integers and depend on the permutation $\{a\}$. Since the number of permutations is $5! = 120$, we cannot explicitly write them down here. What is important is that all the matrix elements are either of the standard form $\langle \dots \rangle_S$ with the constant coefficients c or of the Fermi interaction form $\langle \dots \rangle_F$ with the c^F coefficients.

The ${}^2P_{1/2}$ and ${}^2P_{3/2}$ wave functions are constructed using Clebsch-Gordan coefficients. Expectation values with these wave functions can be reduced to spinless expressions with an algebraic prefactor K_J for $J = 1/2$ and $3/2$. Namely, for an operator Q , the first-order matrix elements with an auxiliary notation $\{K_{1/2}, K_{3/2}\}$ take the form

$$\langle \Phi | Q | \Phi \rangle = \{1, 1\} \langle \phi^i | Q | \phi^i \rangle_S, \quad (21)$$

$$\langle \Phi | \sum_c \vec{\sigma}_c \cdot \vec{Q}_c | \Phi \rangle = \{1, -1/2\} \iota \epsilon^{ijk} \langle \phi^i | Q^j | \phi^k \rangle_F, \quad (22)$$

$$\frac{1}{J(J+1)} \langle \Phi | \vec{J} \cdot \sum_c \vec{\sigma}_c Q_c | \Phi \rangle = \{-2/3, 2/3\} \langle \phi^i | Q | \phi^i \rangle_F, \quad (23)$$

$$\frac{1}{J(J+1)} \langle \Phi | \vec{J} \cdot \vec{Q} | \Phi \rangle = \{-2/3, -1/3\} \iota \epsilon^{ijk} \langle \phi^i | Q^j | \phi^k \rangle_S, \quad (24)$$

$$\frac{1}{J(J+1)} \langle \Phi | J^i \sum_c \sigma_c^j Q_c^{ij} | \Phi \rangle = \{4/3, -2/15\} \times \langle \phi^i | Q^{ij} | \phi^j \rangle_F, \quad (25)$$

$$\frac{2}{(2J+3)(J+1)} \langle \Phi | J^i J^j Q^{ij} | \Phi \rangle = \{0, -1/5\} \times \langle \phi^i | Q^{ij} | \phi^j \rangle_S. \quad (26)$$

The above spin reduced matrix elements involve only scalars built of spatial variables \vec{r}_a , and therefore they all can easily be expressed by Gaussian type integrals.

NUMERICAL CALCULATIONS AND RESULTS

In the numerical calculations we employed the ECG basis functions of progressively doubled size from 1024 to 8192 terms for the B atom, and from 512 to 4096 terms for the B^+ ion. The nonlinear parameters were optimized variationally with respect to E_0 until the energy reached stability in a desired number of digits. The sequence of energies obtained for consecutive basis sets enables estimation of the basis truncation error. The convergence for the 2^2P and 3^2S levels of B, and the 2^1S state of the B^+ ion is presented in Table I. The variational energies obtained from the largest expansion are lower than the best results previously reported in [23, 24].

TABLE I: Convergence of the clamped nucleus energy E_0 (in a.u.) of the ground (2^2P) and the lowest excited (3^2S) states of boron atom. At the bottom, several results reported in literature are given.

Basis size	2^2P	3^2S	$2^1S(B^+)$	Ref.
1024	-24.653 755 522	-24.471 358 195	-24.348 883 829 93	
2048	-24.653 844 393	-24.471 386 316	-24.348 884 352 93	
4096	-24.653 864 204	-24.471 391 933	-24.348 884 458 05	
8192	-24.653 867 537	-24.471 393 366	—	
∞	-24.653 868 05(45)	-24.471 393 68(32)	-24.348 884 479(14)	
5100	-24.653 866 08(250)	-24.471 393 06(50)		[24]
Full CI	-24.653 837 33			[25]
10000			-24.348 884 446(35)	[23]

In a similar way, i.e. from the convergence with the growing basis set size, the truncation errors of the expectation values of various operators were estimated. Particular care was taken for the singular or nearly singular operators

$(p_a^4, \delta^3(r_a), \delta^3(r_{ab}), P(r_{ab}^{-3}))$, which exhibit a slow numerical convergence of their mean values. This undesirable effect is particularly pronounced for the ECG functions having improper short-distance behavior. The solution is to employ

the regularized matrix elements following Drachman's recipes [26]. Previously [22], this approach enabled the accuracy of the expectation values to be increased by several orders of magnitude.

The expectation values of all the operators involved in the determination of the fine structure states energy are collected in Table II. All the entries are accompanied by their estimated uncertainty. Table III contains the α -expansion components and the final values of the measurable quantities: the $3^2S_{1/2} - 2^2P_{1/2}$ transition energy, the fine-structure splitting, and the ground state ionization potential for the most abundant ^{11}B isotope of the boron atom. In the table, the theoretical predictions are compared with recent calculations [27–29] and with the experimental values collected by Kramida and Ryabtsev [30]. The agreement of the new values with the experimental results is apparent and the remaining discrepancies are consistent with estimated uncertainties due to the approximate value of the Bethe logarithm and due to neglected higher-order $\mathcal{O}(\alpha^6)$ corrections. In contrast, significant differences are observed with all the previous calculations. Although none of the cited theoretical values carries uncertainty, it is clear that the number of digits quoted there is by far too high. One may conclude, that the standard configuration interaction (CI), multiconfiguration Dirac-Fock (MCDF) or cou-

pled clusters (CC) methods based on one-electron functions are not capable of supplying results with controlled precision.

The numerical results for the hyperfine splitting are presented in Tables IV and V. The former table collects the expectation values of individual operators comprising the H_{hfs} Hamiltonian and include the Fermi contact, orbital term, spin-dipole term as well as the term describing the interaction of the nuclear electric quadrupole moment with the electric-field gradient produced by electrons. The head of this table presents a relation of the expectation values to the commonly used hyperfine parameters and the corresponding prefactors used in their evaluation. We observe significant discrepancies for individual contributions in Table IV with the results from the previous calculations by Chen [27]. This is particularly pronounced in the case of the Fermi-contact parameter a_c , for which this discrepancy is over 25%. Surprisingly, the differences between Chen's results and the previously established experimental A -hyperfine constants are much smaller (see Tab. V). Moreover, the difference between our result and the experimental values is consistent with the $O(Z\alpha)^2$ unknown relativistic correction, namely it is about 50% of $(Z\alpha)^2$ times the corresponding A or B coefficient. The final values for both the 2^2P levels and both ^{11}B and ^{10}B isotopes are presented in Table V.

TABLE II: Expectation values of various spinless and fine-structure operators for 2^2P and 3^2S states of boron atom. To obtain the mean values for 2^2P_J , the value for 2^2P state has to be multiplied by the relevant $\{K_{1/2}, K_{3/2}\}$ coefficient in curly bracket i.e. $\{1, -\frac{1}{2}\}$ following Eqs. (21) – (26).

Operator	2^2P	3^2S	$2^1S(\text{B}^+)$
H_0	-24.653 868 1(5)	-24.471 393 7(3)	-24.348 884 479(14)
$\vec{p}_a \cdot \vec{p}_b$	0.271 175(2)	0.607 784(3)	0.595 137 52(4)
p_a^4	5 546.924(3)	5 602.919(2)	5598.710 4(3)
$\delta(r_a)$	71.864 97(3)	72.544 82(2)	72.506 327(3)
$\delta(r_{ab})$	3.538 453 2(14)	3.582 111 2(7)	3.577 866 33(12)
$p_a^i \left(\frac{\delta^{ij}}{r_{ab}} + \frac{r_{ab}^i r_{ab}^j}{r_{ab}^3} \right) p_b^j$	2.171 606(3)	2.995 875(3)	3.025 198 47(14)
$\frac{\vec{r}_a}{r_a^3} \times \vec{p}_a \cdot \vec{\sigma}_a$	-1.494 336(5)	—	—
$\frac{\vec{r}_{ab}}{r_{ab}^3} \times \vec{p}_a \cdot \vec{\sigma}_a$	-2.855 953(3)	—	—
$\frac{\vec{r}_{ab}}{r_{ab}^3} \times \vec{p}_b \cdot \vec{\sigma}_a$	0.568 459(4)	—	—
$P(r_{ab}^{-3})$	-27.874 22(6)	-29.391 67(4)	-29.459 453 0(3)
$\ln k_0$	6.195(5) ^a	6.195(5) ^a	6.194 4(9) ^b

^a estimated from $\ln k_0[2^1S(\text{B}^+)]$

^b Ref. [23]

CONCLUSIONS

We calculated the energy levels, isotope shifts, and fine and hyperfine structure in the atomic boron with numerical pre-

cision of a few parts per million. We demonstrated that the majority of the previous calculations were not as accurate as claimed—instead of five to six digits only the first two were significant. This is particularly apparent for the fine structure

TABLE III: Components of the $3^2S_{1/2} - 2^2P_{1/2}$ transition energy, the fine structure splitting, and the ionization potential (IP) for ^{11}B atom and of the ground level energy for $^{11}\text{B}^+$. For comparison, previous theoretical predictions and the experimental results are given at the bottom. All entries in cm^{-1} .

Component	$3^2S_{1/2} - 2^2P_{1/2}$	$2^2P_{3/2} - 2^2P_{1/2}$	IP($2^2P_{1/2}$)	$2^1S_0(\text{B}^+)$
$m\alpha^2$	40 048.50(5)		66 936.15(5)	-5 343 962.445(3)
$m\alpha^2\eta$	1.686(0)		0.207 6(0)	272.846(0)
$m\alpha^4$	-12.424(3)	15.287 8(1)	-10.131(2)	-1410.050(0)
$m\alpha^5$	1.66(24)		1.59(20)	173.68(4)
$m\alpha^6$	0.10(3)	0.000(2)	0.10(3)	10.851(0)
Total	40 039.52(24)	15.288(2)	66 927.91(21)	
Theory, 2011 [24] ^a	40 049.887(200)			
Theory, 2015 [27]	40 008.67	15.523		
Theory, 2012 [29]	39 892.82	19.75	66 886.58	
Theory, 2004 [28]	40 005.27	15.39		
Experiment [30]	40 039.656(3)	15.287(3)	66 928.036(22)	

^a without relativistic and QED corrections

TABLE IV: Expectation values of hyperfine splitting operators for 2^2P state of boron atom $^{\infty}\text{B}$, in relation to standard hyperfine parameters.

Reference	$\vec{\sigma}_a \delta^3(r_a) (\equiv \frac{a_c}{4\pi})$	$\frac{\vec{r}_a}{r_a^3} \times \vec{p}_a (\equiv -2 a_l)$	$\frac{\sigma_a^i}{r_a^3} \left(\delta^{ij} - 3 \frac{r_a^i r_a^j}{r_a^2} \right) (\equiv 10 a_{sd})$	$\frac{1}{r_a^3} \left(\delta^{ij} - 3 \frac{r_a^i r_a^j}{r_a^2} \right) (\equiv 5 b_q)$
This work	0.007 536(2)	-1.560 155(5)	-1.677 193(11)	-1.417 48(12)
Theory, 2015 [27] ^a	0.010 13	-1.557 6	-1.684	-1.400 5
Theory, 1993 [31] ^a	0.006 828	-1.561 4	-1.672	-1.422

^a values calculated for ^{11}B

TABLE V: Hyperfine splitting parameters (in MHz) for the ground state 2^2P state; relativistic and finite mass corrections are not included so the uncertainties are purely numerical; magnetic moments are [32] $\mu(^{11}\text{B}) = 2.688 648 9(10) \mu_N$ and $\mu(^{10}\text{B}) = 1.800 644 78(6) \mu_N$.

Reference	$A_{1/2}(^{11}\text{B})$	$A_{3/2}(^{11}\text{B})$	$B_{3/2}(^{11}\text{B})$	$A_{1/2}(^{10}\text{B})$	$A_{3/2}(^{10}\text{B})$	$B_{3/2}(^{10}\text{B})$
This work	365.710 1(18)	73.395 3(15)	2.704 0(4)	122.462 4(6)	24.577 8(6)	5.635 1(8)
Theory, 2015 [27]	365.91	73.41	2.675	122.21	24.92	5.575
Theory, 2012 [29]	373.3	72.7				
Theory, 1996 [33]	366.1	73.24				
Experiment, 1960 [34]	366.076 5(15)			122.585 1(9)		
Experiment, 1972 [35]		73.349 6(4)	2.692 7(10)			

splitting and for the Fermi contact interaction, the last one being exceptionally small for the $2P$ ground state. The smallness of the Fermi contact term makes the hyperfine splitting insensitive to the not-well-known nuclear finite size effects, thus the comparison with experimental hfs will be a good test of the atomic computational methods. Moreover, the precise value for the mass polarization correction (see Tab. II) permits the accurate determination of the isotope shift in the $2P - 3S$ transition, which paves the way for determination of the nu-

clear charge radius of the proton halo in the ^8B nucleus, as we have already demonstrated for the beryllium atom [8].

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