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^{7}Be(p, γ)^{8}B S-factor from ab initio wave functions

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Abstract

Nuclear structure of ^{7}Be, ^{8}B and ^{7,8}Li is studied within the ab initio no-core shell model (NCSM). Starting from the high-precision CD-Bonn 2000 nucleon–nucleon (NN) interaction, wave functions of ^{7}Be and ^{8}B bound states are obtained in basis spaces up to $10\hbar\Omega$ and used to calculate channel cluster form factors (overlap integrals) of the ^{8}B ground state with ^{7}Be + p. Due to the use of the harmonic oscillator (HO) basis, the overlap integrals have incorrect asymptotic properties. We fix this problem in two alternative ways. First, by a Woods–Saxon (WS) potential solution fit to the interior of the NCSM overlap integrals. Second, by a direct matching with the Whittaker function. The corrected overlap integrals are then used for the ^{7}Be(p, γ)^{8}B S-factor calculation. We study the convergence of the S-factor with respect to the NCSM HO frequency and the model space size. Our S-factor results are in agreement with recent direct measurement data.

PACS: 21.60.Cs; 21.30.Fe; 24.10.Cn; 25.40.Lw; 27.20.+n

The ^{7}Be(p, γ)^{8}B capture reaction serves as an important input for understanding the solar neutrino flux [1]. Recent experiments have determined the neutrino flux emitted from ^{8}B with a precision of 9% [2]. On the other hand, theoretical predictions have uncertainties of the order of 20% [3,4]. The theoretical neutrino flux depends on the ^{7}Be(p, γ)^{8}B S-factor. Many experimental and theoretical investigations studied this reaction. Experiments were performed using direct techniques with proton beams and ^{7}Be targets [5–7] as well as by indirect methods when a ^{8}B beam breaks up into ^{7}Be and proton [8,9]. Theoretical calculations needed to extrapolate the measured S-factor to the astrophysically relevant Gamow energy were performed with several methods: the R-matrix parametrization [10], the potential model [11–13], and the microscopic cluster models [14–16].

In this Letter, we present the first calculation of the ^{7}Be(p, γ)^{8}B S-factor starting from ab initio wave functions of ^{8}B and ^{7}Be. It should be noted that the aim of ab initio approaches is to predict correctly absolute cross sections (S-factors), not just relative cross sections. We apply the ab initio no-core shell model (NCSM) [17]. In this method, one considers nucleons interacting by high-precision nucleon–nucleon (NN) potentials. There are no adjustable or fitted parameters. We study the binding energies and other nuclear structure properties of ^{7}Be, ^{8}B as well as ^{7,8}Li, and calculate overlap integrals for the ^{8}B and ^{7}Be bound states. Due to the use of the harmonic-oscillator (HO) basis, we have to correct the asymptotic behavior of the NCSM overlap integrals. This is done in two alternative ways. First, by fitting Woods–Saxon (WS) potential solutions to the interior part of the NCSM overlap integrals under the constraint that the experimental ^{7}Be + p threshold energy is reproduced. Second, by a direct matching with the Whittaker function. The corrected overlap integrals are then utilized to calculate the ^{7}Be(p, γ)^{8}B S-factor as well as momentum distributions in stripping reactions.

Our calculations for both $A = 7$ and $A = 8$ nuclei were performed using the high-precison CD-Bonn 2000 NN potential [18] in model spaces up to $10\hbar\Omega$ ($N_{\max} = 10$) for a wide range of HO frequencies. We then selected the optimal HO frequency corresponding to the ground-state (g.s.) energy minimum in the

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Table 1
The ^{7}Be and ^{7}Li $\frac{3}{2}^-\,\frac{1}{2}$ (^{8}B and ^{8}Li 2^+1) g.s. energies (in MeV), point-proton radii (in fm), quadrupole (in e fm^2) and magnetic (in μ_N) moments and $\frac{1}{2}^-_1 \to \frac{3}{2}^-_1$ ($1^+_1 \to 2^+_1$) M1 transitions (in μ_N^2) obtained within the NCSM for the HO frequency of $\hbar\Omega = 12$ MeV. Experimental values are from Refs. [19,20]

N_{max}	CD-Bonn 2000				
	$\lvert E_{gs}\rvert$	r_p	Q	μ	B(M1)
^{7}Be					
6	33.302	2.311	−4.755	−1.150	3.192
8	33.841	2.324	−4.975	−1.151	3.145
10	33.972	2.342	−5.153	−1.141	3.114
12	33.881	2.365			
Expt.	37.6004(5)	2.36(2)		−1.398(15)	3.71(48)
^{7}Li					
6	34.951	2.149	−2.717	+3.027	4.256
8	35.494	2.156	−2.866	+3.020	4.188
10	35.623	2.168	−3.001	+3.011	4.132
12	35.524	2.188	−3.130		
Expt.	39.245	2.27(2)	−4.06(8)	+3.256	4.92(25)
^{8}B					
6	31.772	2.436	+5.218	+1.463	3.498
8	32.258	2.463	+5.420	+1.455	3.506
10	32.367	2.487	+5.636	+1.455	3.490
12	32.284	2.520			
Expt.	37.7378(11)	2.45(5)	(+)6.83(21)	1.0355(3)	9.1(4.5)
^{8}Li					
6	35.352	2.139	+2.588	+1.238	4.454
8	35.834	2.139	+2.690	+1.243	4.428
10	35.928	2.145	+2.784	+1.241	4.393
12	35.820	2.161			
Expt.	41.277	2.26(2)	+3.27(6)	+1.654	5.01(1.61)

$10\hbar\Omega$ space, here $\hbar\Omega = 12$ MeV, and performed a $12\hbar\Omega$ calculation to obtain the g.s. energy and the point-nucleon radii. The overlap integrals as well as other observables were, however, calculated only using wave functions from up to $10\hbar\Omega$ spaces. The g.s. energies, radii and electromagnetic observables are summarized in Table 1. Note that the CD-Bonn 2000 underbinds ^{7}Be, ^{8}B and ^{7,8}Li by about 3–5 MeV and predicts ^{8}B unbound, contrary to experiment. This suggests that the three-nucleon interaction is essential to accurately reproduce the experimental threshold. However, since the HO basis has the incorrect asymptotic behavior in the first place, we make use of only the interior part of our ab initio wave functions, which are likely unaffected by mild variations in the threshold value. Concerning the excitation energies, we obtained the same level ordering for ^{7}Be and ^{7}Li. Our CD-Bonn 2000 ordering is in agreement with experiment for the 9 lowest levels in ^{7}Li. In ^{7}Be, the experimental $7/2^-_2$ and $3/2^-_2$ levels are reversed compared to our results and to the situation in ^{7}Li. While for the magnetic moments and M1 transitions we obtained a very small dependence of the calculated values on the HO frequency or the basis size, the radii and quadrupole moments in general increase with increasing basis size and decreasing frequency. The fastest convergence for the radii and quadrupole moment occurs at a smaller HO frequency. In our calculations with $\hbar\Omega = 11$ and 12 MeV, the radii are close to experimental values.

Table 2
The NCSM $\langle ^8\mathrm{B}|^7\mathrm{Be}+\mathrm{p}\rangle$ spectroscopic factors

CD-Bonn 2000		^{7}Be + p $I^\pi_1(l,j)$		
$\hbar\Omega$ [MeV]	N_{max}	$\frac{3}{2}^-(1,\frac{3}{2})$	$\frac{3}{2}^-(1,\frac{1}{2})$	$\frac{1}{2}^-(1,\frac{3}{2})$
11	8	0.967	0.116	0.280
11	10	0.959	0.111	0.275
12	6	0.978	0.107	0.287
12	8	0.969	0.103	0.281
12	10	0.960	0.102	0.276
14	8	0.967	0.085	0.284
14	10	0.958	0.085	0.280

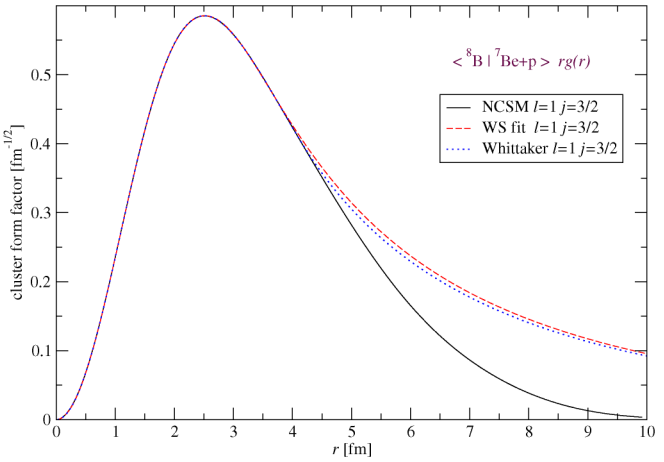

Fig. 1. Overlap integral, $rg(r)$, for the g.s. of ^{8}B with the g.s. of ^{7}Be plus proton. For further details see the text.

From the obtained ^{8}B and ^{7}Be wave functions, we calculate the channel cluster form factors $g^{A\lambda J}_{(l\frac{1}{2})j;A-1\alpha I_1}(r)$ following Ref. [21]. Here, $A = 8$, l is the channel relative orbital angular momentum and $\vec{r} = [\frac{1}{A-1}(\vec{r}_1 + \vec{r}_2 + \cdots + \vec{r}_{A-1}) - \vec{r}_A]$ describes the relative distance between the proton and ^{7}Be. A conventional spectroscopic factor is obtained as $S^{A\lambda J}_{(l\frac{1}{2})j;A-1\alpha I_1} = \int dr\, r^2 |g^{A\lambda J}_{(l\frac{1}{2})j;A-1\alpha I_1}(r)|^2$. Our selected spectroscopic factor results are summarized in Table 2. We note a very weak dependence of the spectroscopic factors on either the basis size or the HO frequency.

The dominant p-wave $j = 3/2$ overlap integral for the ^{8}B and ^{7}Be ground states obtained using the CD-Bonn 2000 NN potential in the $10\hbar\Omega$ model space and the HO frequency of $\hbar\Omega = 12$ MeV is presented in Fig. 1 by the full line. Despite the fact that a very large basis was employed, it is apparent that the overlap integral is nearly zero at about 10 fm. This is a consequence of the HO basis asymptotics. The proton capture on ^{7}Be to the weakly bound g.s. of ^{8}B associated dominantly by E1 radiation is a peripheral process. Consequently, the overlap integral with an incorrect asymptotics cannot be used to calculate the S-factor. We expect, however, that the interior part of the overlap integral is realistic. It is then straightforward to correct its asymptotics. One possibility we explored utilizes solutions of a Woods–Saxon (WS) potential. In particular, we performed a least-square fit of a WS potential solution to the interior of the NCSM overlap in the range of 0–4 fm. The WS potential

Table 3
Parameters of the WS potentials obtained in the fits to the interior part of the NCSM $\langle {}^8\mathrm{B}(2^+_{\mathrm{gs}})|{}^7\mathrm{Be}(I^\pi_1)+\mathrm{p}(l,j)\rangle(r)$ overlap functions

CD-Bonn 2000 $10\hbar\Omega$ $\hbar\Omega = 12$ MeV							
$I^\pi_1\,(l,j)$	V_0	R_0	a_0	V_{ls}	R_{ls}	a_{ls}	R_{C}
$\frac{3}{2}^-\,(1,\frac{3}{2})$	−51.037	2.198	0.602	−9.719	2.964	0.279	2.198
$\frac{3}{2}^-\,(1,\frac{1}{2})$	−45.406	2.613	0.631	−8.414	2.243	0.366	2.613
$\frac{1}{2}^-\,(1,\frac{3}{2})$	−49.814	2.235	0.553	−17.024	3.080	0.338	2.235
Scattering state [22]							
	−42.2	2.391	0.52	−9.244	2.391	0.52	2.391

parameters were varied in the fit under the constraint that the experimental separation energy of ^{7}Be+p, $E_0 = 0.137$ MeV, was reproduced. In this way we obtain a perfect fit to the interior of the overlap integral and a correct asymptotic behavior at the same time. The result is shown in Fig. 1 by the dashed line.

Another possibility is a direct matching of logarithmic derivatives of the NCSM overlap integral and the Whittaker function: $\frac{d}{dr}\ln(r g_{lj}(r)) = \frac{d}{dr}\ln(C_{lj} W_{-\eta,l+1/2}(2k_0 r))$, where η is the Sommerfeld parameter, $k_0 = \sqrt{2\mu E_0}/\hbar$ with μ the reduced mass and E_0 the separation energy. Since asymptotic normalization constant (ANC) C_{lj} cancels out, there is a unique solution at $r = R_m$. For the discussed overlap presented in Fig. 1, we found $R_m = 4.05$ fm. The corrected overlap using the Whittaker function matching is shown in Fig. 1 by a dotted line. In general, we observe that the approach using the WS fit leads to deviations from the original NCSM overlap starting at a smaller radius. In addition, the WS solution fit introduces an intermediate range from about 4 fm to about 6 fm, where the corrected overlap deviates from both the original NCSM overlap and the Whittaker function. Perhaps, this is a more realistic approach compared to the direct Whittaker function matching. In any case, by considering the two alternative procedures we are in a better position to estimate uncertainties in our S-factor results.

In the end, we re-scale the corrected overlap functions to preserve the original NCSM spectroscopic factors (Table 2). In general, we observe a faster convergence of the spectroscopic factors than that of the overlap functions. The corrected overlap function should represent the infinite space result. By re-scaling a corrected overlap function obtained at a finite $N_{\max}$, we approach faster the infinite space result. The same procedure is applied to other relevant channels. In Table 3, we show examples of the fitted WS parameters obtained in the two p-wave channels together with parameters corresponding to a p-wave channel with ^{7}Be in the first excited state ($E_0 = 0.57$ MeV). We use the definition of the WS potential as given, e.g. in Eqs. (5)–(7) of Ref. [23]. Typically, the central potential parameters R_0, a_0 are well constrained in the fit, while the spin-orbit potential parameters are obtained with some uncertainty. The range used in the least-square fit is not arbitrary but varies from channel to channel. The aim is to use as large range as possible, while at the same time preserve the NCSM overlap integral as accurately as possible in that range. Concerning the above discussed example (dashed line in Fig. 1), we note that extending the range beyond 4 fm leads to a worse fit.

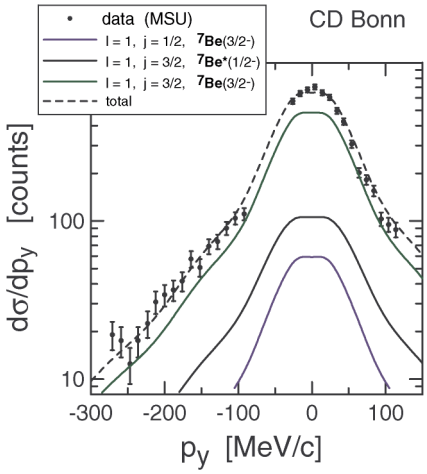

Fig. 2. Inclusive transverse-momentum distribution for the ^{7}Be residue in the ^{9}Be(^{8}B, ^{7}Be)X reaction at 41 MeV/A [25].

Table 4
Cross sections for the proton-removal reactions $^8\mathrm{B} + {}^9\mathrm{Be}$ at 41 MeV/nucleon (MSU) and $^8\mathrm{B} + {}^{12}\mathrm{C}$ at 936 MeV/nucleon (GSI). The calculated total inclusive (excited state) cross sections, in mb, are given by $\sigma^{(\mathrm{th})}_{\mathrm{inc}}$ ($\sigma^{(\mathrm{th})}_{\mathrm{exc}}$)

CD-Bonn 2000 $10\hbar\Omega$ $\hbar\Omega = 12$ MeV WS fit				
	$\sigma^{(\mathrm{exp})}_{\mathrm{inc}}$	$\sigma^{(\mathrm{th})}_{\mathrm{inc}}$	$\sigma^{(\mathrm{exp})}_{\mathrm{exc}}$	$\sigma^{(\mathrm{th})}_{\mathrm{exc}}$
MSU	–	82.96	–	15.31
GSI	94 ± 9	99.66	12 ± 3	16.36

The momentum distributions in break-up reactions present a direct test of the corrected NCSM overlap integrals. We compared our calculations performed as described in Ref. [24] to two sets of experimental data. First, to an experiment performed at MSU for the transverse momentum distributions of ^{7}Be fragments from the reaction $^8\mathrm{B} + {}^9\mathrm{Be}$ at 41 MeV/A [25]. Second, for the longitudinal momentum distributions, the data were taken from a GSI experiment [26] which measured gamma rays in coincidence with ^{7}Be residues in the reaction $^8\mathrm{B} + {}^{12}\mathrm{C}$ at 936 MeV/A. Some of our results are summarized in Fig. 2 and Table 4. A good agreement with experiment is observed. As the MSU data is given in arbitrary units, we multiplied the contributions from each channel by the same factor so that their sum reproduces the maximum of the experimental distribution.

The S-factor for the reaction $^7\mathrm{Be}(\mathrm{p},\gamma)^8\mathrm{B}$ also depends on the continuum wave function, $R^{(c)}_{lj}$. As we have not yet developed an extension of the NCSM to describe continuum wave functions, we obtain $R^{(c)}_{lj}$ for s and d waves from a WS potential model. Since the largest part of the integrand stays outside the nuclear interior, one expects that the continuum wave functions are well described in this way. In order to have the same scattering wave function in all the calculations, we chose a WS potential from Ref. [22] that was fitted to reproduce the p-wave 1^+ resonance in ^{8}B (Table 3). It was argued [11] that such a potential is also suitable for the description of s- and d-waves. We note that the S-factor is very weakly dependent on the choice of the scattering-state potential (using our fitted potential for the scattering state instead changes the S-factor by less than 1.5 eV b at 1.6 MeV with no change at 0 MeV).

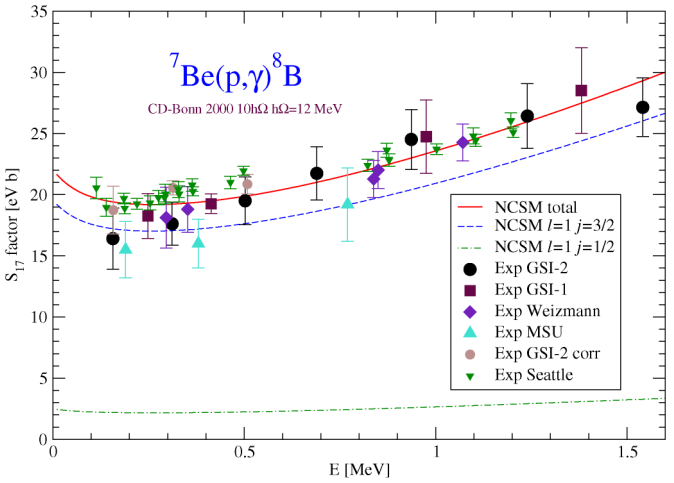

Fig. 3. The ^{7}Be(p, γ)^{8}B S-factor obtained using the NCSM cluster form factors with corrected asymptotics by the WS solution fit. Experimental values are from Refs. [6,7,9].

Table 5
The calculated ^{7}Be(p, γ)^{8}B S-factor, in eV b, at the energy of 10 keV. Two ways of correcting the NCSM overlap asymptotics, by the Woods–Saxon potential solution fit (WS) and by a direct Whittaker function matching (Whit), are compared. The asymptotic normalization constants, in fm$^{-1/2}$, correspond to the Whittaker function matching case

CD-Bonn 2000					
$\hbar\Omega$ [MeV]	$N_{\max}$	$S_{17}^{\rm WS}(10)$	$S_{17}^{\rm Whit}(10)$	$C_{1,3/2}$	$C_{1,1/2}$
15	6	17.80	16.81	0.647	0.195
15	8	18.87	17.58	0.660	0.206
15	10	19.81	18.33	0.672	0.216
14	10	20.21	18.78	0.680	0.220
13	10	21.02	19.64	0.692	0.234
12	6	21.24	19.75	0.693	0.240
12	8	21.14	19.96	0.696	0.242
12	10	21.66	20.45	0.704	0.247
11	6	22.38	21.30	0.715	0.261
11	8	23.04	21.33	0.715	0.263
11	10	23.06	21.60	0.720	0.262
NCSM S_{17}(10 keV)		22.1 ± 1.0			

Fig. 3 shows the astrophysical S-factor for the reaction ^{7}Be(p, γ)^{8}B. We use bound-state wave functions calculated with the CD-Bonn 2000 interaction in the $10\hbar\Omega$ model space and the HO frequency $\hbar\Omega = 12$ MeV. The WS solution fit procedure was employed to correct the asymptotics of the NCSM overlap functions. The S-factor contributions from the dominant $l = 1$, $j = 3/2$ and $j = 1/2$ partial waves are drawn by the dashed lines. The full line is the sum of the two contributions. The experimental data is a compilation of the latest experiments for the S-factor. They include direct, as well as some indirect measurements (Coulomb dissociation). The slope of the curve corresponding to the total S-factor follows the trend of the data. Our result is in a very good agreement with the recent direct measurement data of Ref. [7].

In order to judge the convergence of our S-factor calculation, we performed a detailed investigation of the model-space-size and the HO-frequency dependencies. In Table 5, we summarize our S-factor results at 10 keV. We observe a steady increase of the S-factor with the basis size enlargement for higher frequencies. Contrary to this situation, the calculation using the HO frequency of $\hbar\Omega = 11$ MeV and the WS solution fit shows that the S-factor does not increase any more with increasing $N_{\max}$. We also present the S_{17} and the ANC obtained using the alternative direct Whittaker matching procedure. In general, both procedures lead to basically identical energy dependence with a difference of about 1 to 2 eV b in the S-factor with the smaller values from the direct Whittaker function matching procedure. Results at $\hbar\Omega = 11$ and 12 MeV show very weak dependence on $N_{\max}$, with relative difference between the two methods always in the range of 5 to 8%. The full range of results is covered by $S_{17}(10\ \text{keV}) = 22.1 \pm 1.0$ eV b. We stress that no adjustable parameters were used in our ab initio calculations of the ^{8}B and ^{7}Be bound states. Taking into account that the S-factor is only weakly dependent on the potential model used to obtain the scattering state, we consider our results as the first ab initio prediction of the ^{7}Be(p, γ)^{8}B S-factor, in particular of its normalization.

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