Ab initio calculations for Be-isotopes with JISP16

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Abstract. We present recent results from no-core configuration interaction calculations for $^8$Be, $^{10}$Be, and $^{12}$Be using the phenomenological two-body interaction JISP16. We calculate the binding energies of the ground state and the excitation energies of the low-lying positive-parity states. We discuss the contributions from the proton and neutron intrinsic spin and orbital motion to the total spin for several states, and use this to identify states which may be dominated by $\alpha$-cluster configurations. In addition, we also calculate other observables such as dipole and quadrupole moments, as well as transition rates for select E2 transitions.

1. No-Core Configuration Interaction approach

Configuration Interaction (CI) methods have been used in recent years to make increasingly accurate large scale ab initio calculations in nuclear structure, see e.g. Refs. [1, 2] and references therein. In this method, the many-body Schrödinger equation

$$H \Psi_A(r_1, \ldots, r_A) = E_i \Psi_A(r_1, \ldots, r_A)$$

becomes a large sparse matrix problem with eigenvalues $E_i$. Improved algorithms to construct this matrix and to determine its lowest eigenstates, as well as efficient use of increasing computational resources are critical for these successes [3, 4, 5, 6, 7, 8].

In the No-Core CI (NCCI) approach [1, 2, 9] the wavefunction $\Psi$ of a nucleus consisting of $A$ nucleons (protons and neutrons) is expanded in an $A$-body basis of Slater determinants $\Phi_k$ of single-particle wavefunctions $\phi_{nljm}(\vec{r})$

$$\Psi(r_1, \ldots, r_A) = \sum c_k \Phi_k(r_1, \ldots, r_A),$$

with $\Phi_k(r_1, \ldots, r_A) = A[n_i, l_j, m_i(r_1) \phi_{n_2 l_2} m_2(r_2) \ldots \phi_{n_A l_A} m_A(r_A)]$ and $A$ the antisymmetrization operation. Conventionally, one uses a harmonic oscillator (HO) basis for the single-particle wavefunctions, but it is straightforward to extend this approach to a more general single-particle basis [10]. The single-particle wavefunctions are labelled by the quantum numbers $n$, $l$, $j$, and $m$, where $n$ and $l$ are the radial and orbital HO quantum numbers, with $N_i = 2n_i + l_i$ the number of HO quanta; $j$ is the total single-particle spin, and $m$ its projection along the z-axis. The many-body basis states $\Phi_k$ have well-defined total spin-projection, which is simply the sum of $m_i$ of the single-particle states, $M = \sum m_i$ (hence the name $M$-scheme), but they do not have a well-defined total spin $J$. Some of the benefits of this scheme is that it is straightforward to implement, and that in two runs (one for positive and one for negative parity), we get the complete low-lying spectrum, including the ground state, even if the spin of the ground state is not known a priori.
In a complete basis, this method would give exact results for a given potential. However, practical calculations can only be done in a finite-dimensional truncation of a complete basis. Different truncation schemes have different convergence rates: Full Configuration Interaction (FCI) employs a widely-know truncation in which all many-body basis states are retained that can be constructed from a finite set of single-particle states. However, this truncation has a rather slow convergence rate (as function of the dimensionality of the basis space) in typical NCCI calculations [11, 12]. The so-called $N_{\text{max}}$ truncation, which is a truncation on the total number of HO quanta in the many-body basis: $\sum N_i \leq N_0 + N_{\text{max}}$, is generally much more efficient for NCCI calculations. Here, $N_i$ is the number of quanta of each single-particle state in the many-body basis state; $N_0$ is the minimal number of quanta for that nucleus; and $N_{\text{max}}$ is the truncation parameter. Furthermore, for HO single-particle states, this truncation leads to an exact factorization of the center-of-mass wavefunction and the relative wavefunction [1, 2, 10, 13].

2. Recent results for Be isotopes with JISP16
Here we present new results for the Beryllium isotopes using JISP16 [14], which is a phenomenological nonlocal $NN$-interaction written as a finite matrix in a HO basis. It is constructed to reproduce the available $NN$ scattering data using the $J$-matrix inverse scattering approach. In addition, phase-equivalent transformations have been used to modify its off-shell properties in order to achieve a good description of selected states in light nuclei [14]. It gives a good description of most narrow states in light nuclei up to about $A = 12$ [15, 16] without additional three-nucleon forces. For our calculations we use the code MFDn [4, 5, 6, 7] which has been demonstrated to scale to over 200,000 cores, and we consider basis spaces with dimensions up to 3.3 billion basis states, and nearly 4 trillion nonzero matrix elements.

Because of the variational principle, any result for the ground state energy in a finite basis forms a strict upper bound for the exact ground state energy. Indeed, our calculated energies in finite bases are all above the experimental ground state energies, see Fig. 1. With an exponential extrapolation [15] we obtain No-Core Full Configuration (NCFC) results for the ground state energies (with numerical error bars due to the extrapolation uncertainties) that are in general much closer to the experimental data than these variational upper bounds. It turns out that with JISP16 all Be-isotopes are underbound [3]: the light isotopes, $^6\text{Be}$ and $^7\text{Be}$, by a fraction of an MeV, and the neutron-rich isotopes $^{13}\text{Be}$ and $^{14}\text{Be}$ by about 5 MeV. Nevertheless, the overall pattern of the ground state energies is in reasonable agreement with the data [17].
2.1. Results for $^8$Be

In Fig. 2 we show the ground state energy of $^8$Be as function of the basis parameter $\hbar \omega$ for a range of different $N_{\text{max}}$ values, as well as the extrapolation [15] to the infinite basis using results at three consecutive $N_{\text{max}}$ values and fixed $\hbar \omega$, as indicated in the legend. Near the minimum of the ground state energy the convergence appears to be reasonable, with an estimated error (due to the extrapolation) of about 0.3 MeV in the ground state energy. Note that both our calculated and the experimental ground state energies are above the threshold for two $\alpha$-particles: we are dealing with a (narrow) resonance, rather than a true bound state.

JISP16 does give the correct ground state energy for an $\alpha$-particle [14, 15]. Hence we know that in the infinite basis space, the energy of the lowest state should be that of two $\alpha$-particles.

On the other hand, our extrapolated ground state energy is about 1 MeV above the threshold for two $\alpha$-particles. We appear to have 'pseudo-convergence' to a resonance which is above the two-$\alpha$ threshold. This could explain why our extrapolated ground state energy still has a significant and systematic dependence on the HO parameter $\hbar \omega$. Nevertheless, the point proton rms radius trends towards a value of about 2.3 fm, but with a large dependence on $\hbar \omega$, see Fig. 3. Again, this appears to be 'pseudo-convergence', since we know that in the infinite basis space, the lowest state is that of two $\alpha$-particles, and hence the radius should go to infinity.

Despite the fact that the ground state is well above the threshold for two $\alpha$-particles, the spectrum of the positive parity states looks in reasonable agreement with the data [18], see Fig. 4. The excitation energies of the two lowest excited states, the $2^+$ and $4^+$ states, are very well converged, and agree with the experimental values. Although neither the quadrupole moments nor the B(E2)'s are converged in these basis spaces, the ratio of $Q_{4^+}/Q_{2^+}$, as well as the ratio's B(E2;2$^+ \rightarrow 0^+$)/$Q_{2^+}^2$ and B(E2;4$^+ \rightarrow 2^+$)/$Q_{2^+}^2$ are in qualitative agreement with a rotational model [19, 20]. Furthermore, more than 95% of their total spins comes from the proton and neutron orbital motion, whereas the proton and neutron intrinsic spin contributes less than 5%. This is all consistent with a picture of these two states being rotational states of the ground state, and their internal structure being dominated by two $\alpha$-cluster configurations.

Next we have several pairs of states with the same spin: a pair of $2^+$, $1^+$, and $3^+$ states, with the lower having approximately isospin $T = 1$, and the higher one having approximately $T = 0$. And finally a $4^+$, $T = 0$ appears at about 20 MeV, with a similar excitation energy as the higher of the two $3^+$ states. All of these states are in reasonable agreement with the data, but not as well converged as the lowest $2^+$ and $4^+$ states. None of these states appear to have an $\alpha$-cluster configuration.
structure: the proton and neutron intrinsic spins contribute at least 20% to the total spin for each of these states.

In addition, we see in Fig. 4 two states that are likely 'continuum states': a 0\(^+\) and a 2\(^+\) state (both isospin 0) which appear in the largest model space calculations, \(N_{\text{max}} = 10\) and 12. These states have a very strong, almost linear, \(\hbar \omega\) dependence. The 0\(^+\) is clearly identifiable, since there are no other 0\(^+\) states in the low-lying spectrum, but the 2\(^+\) 'continuum state' interferes with the isospin 0 resonance at about 17 MeV. The point proton rms radius of the 0\(^+\) state increases rapidly with \(N_{\text{max}}\) and shows no signs of convergence, see Fig. 3. Most likely these two states are continuum states, consisting of two unbound \(\alpha\)-particles.

2.2. Results for \(^{10}\text{Be}\)

In contrast to \(^{8}\text{Be}\), \(^{10}\text{Be}\) is a true bound state, well below the threshold of \(^4\text{He} + ^6\text{He}\), as indicated by the dashed line in the left panel of Fig. 5. After the extrapolation to the infinite basis space, we find a binding energy of 64.0(3) MeV for the 0\(^+\) ground state, compared to the experimental value of 64.98 MeV; that is, JISP16 underbinds this state by about 1 MeV.

The first excited state is a 2\(^+\) state, its excitation energy is rapidly converging in our calculations, and in good agreement with the data [18]. The second 2\(^+\) state is not very well converged, but after the extrapolation of the binding energy to the infinite basis its excitation energy is in agreement with the data, given the extrapolation uncertainties. However, the first excited 0\(^+\) is missing from our low-lying spectrum. The excitation energy of the lowest excited 0\(^+\) state is above 10 MeV, even after extrapolating the binding energies. As of yet it is unclear why we do not find a low-lying 0\(^+\); it could be an indication that something is missing in the phenomenological NN interaction, or the structure of that state could be such that it cannot be well represented in HO basis. Note that also in \(^{12}\text{C}\) the lowest excited 0\(^+\) is above 10 MeV with JISP16 [15], whereas experimentally the lowest 0\(^+\) state is around 7.7 MeV (the Hoyle state). It is quite possible that the absence of a low-lying 0\(^+\) in \(^{12}\text{C}\) with this interaction and in these basis spaces is related to the absence of a low-lying 0\(^+\) in \(^{10}\text{Be}\).

The magnetic moment of the lowest 2\(^+\) state is reasonably well converged, \(\mu = 1.7(1) \mu_N\), but that of the second 2\(^+\) is not at all converged — though interestingly, the sum of the magnetic moments of the second and third 2\(^+\) states seems to be converged at \(\mu(2^+_2) + \mu(2^+_3) = 5.5 \mu_N\), while \(\mu(2^+_2)\) ranges from 1.5 to 3 \(\mu_N\) for \(\hbar \omega\) between 20 and 30 MeV at \(N_{\text{max}} = 8\). This is mainly due to variations in the contributions from the proton intrinsic spin: over this range in \(\hbar \omega\) the proton intrinsic spin contributes between 10% and 30% to the total spin of these two states.

![Figure 5](image-url)  
**Figure 5.** Ground state energy of \(^{10}\text{Be}\) (left), and low-lying positive parity spectrum (right).
This suggests that neither the second nor the third $2^+$ state is an $\alpha$-cluster state. Calculations in larger basis spaces are needed to resolve this. On the other hand, the lowest $2^+$ state has a spin decomposition that is reasonably well converged, with more than 70% of the spin coming from the proton orbital motion and more than 20% from the neutron orbital motion, whereas the proton and neutron intrinsic spins contribute each less than 5%. Thus it is conceivable that the first $2^+$ state is dominated by two $\alpha$-cluster configurations plus two neutrons.

Neither the quadrupole moments of the $2^+$ states nor the B(E2)’s from the $2^+$ states to the ground states are converged, but it is clear from our calculations that the quadrupole moment of the first $2^+$ state is negative, around $-4$ to $-6\,\text{fm}^2$, while that of the second $2^+$ state is positive, around $+4$ to $+6\,\text{fm}^2$. This is in qualitative agreement with GFMC calculations using AV18 plus IL7 \[22\]. Furthermore, the B(E2) from the first $2^+$ to the ground state is strong, around 6 to $8\,e^2\text{fm}^4$ in our calculations, whereas that of the second $2^+$ is weak, of the order of $0.1\,e^2\text{fm}^4$ in our calculations. This is in reasonable agreement with recent experiments \[21\]: $\text{B(E2; } 2^+_1 \rightarrow 0^+\text{)} = 9.2(3)\,e^2\text{fm}^4$ and $\text{B(E2; } 2^+_2 \rightarrow 0^+\text{)} = 0.11(2)\,e^2\text{fm}^4$.

### 2.3. Results for $^{12}\text{Be}$

Finally, $^{12}\text{Be}$ is an unstable nucleus with a lifetime of 21 ms. It is a semi-magic nucleus: it has eight neutrons, which closes the $p$-shell. In Fig. 6 we show the ground state energy of $^{12}\text{Be}$ as function of the basis space parameter $\hbar\omega$ for a range of different $N_{\text{max}}$ values, as well as the extrapolation (at fixed $\hbar\omega$) to the infinite basis space. We find a binding energy of 66.9(6) MeV for the $0^+$ ground state, compared to the experimental value of 68.65 MeV. That is, our calculations suggest that JISP16 underbinds this nucleus by almost 2 MeV.

The first excited state is a $2^+$ state, in agreement with experiment (see the right panel of Fig. 6), though the excitation energy appears to be somewhat too large: about 3.1(4) MeV, compared to 2.1 MeV experimentally \[23, 24\]. It is interesting to note that for this $2^+$ state the neutron orbital motion contributes less than 10% to the total spin, and their intrinsic spin less than 2% to the total spin. Most of the spin is carried by the proton orbital motion, with a significant fraction coming from the proton intrinsic spin. This indicates that this state is not dominated by $\alpha$-clustering. Furthermore, this $2^+$ state has a large B(E2) to the ground state, of the order of 6 to $10\,e^2\text{fm}^4$, in agreement with the experimental value of $8.0(3.0)\,e^2\text{fm}^4$ \[24\].

The next excited state in the calculated spectrum is a $0^+$, but this state is not very well converged: its excitation energy drops significantly as $N_{\text{max}}$ increases. An exponential extrapolation of the binding energy of this state suggests that it has an excitation energy of about
3 MeV in the limit of an infinite basis space, but with a rather large extrapolation uncertainty. Although its (extrapolated) excitation energy agrees with data, its B(E2) strength to the first excited \(2^+\) state is more than an order of magnitude too small compared to experiment: we find a B(E2) strength that is less than \(0.2 e^2 fm^4\), compared to the experimental value of \(7.0(6) e^2 fm^4\) \cite{Shimoura2007}. Of course, as the energy of this \(0^+\) state gets closer to that of the ground state with increasing \(N_{\text{max}}\), there may be more mixing between these two states, which could strongly influence their B(E2) transition strengths; in addition there are also higher excited \(2^+\) states that are not yet converged, with decreasing excitation energies as \(N_{\text{max}}\) increases, which may or may not mix with the first excited \(2^+\) state.

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