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BRIEF REPORTS

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Study of the electronic rearrangement induced by nuclear transmutations: A *B*-spline approach applied to the β decay of ^{6}He

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The electronic rearrangement resulting from the β decay of ^{6}He has been calculated in the framework of the sudden approximation using a numerical B-spline basis set approach. We have calculated the excitation probabilities to the final discrete states of ^{6}Li$^+$ (including to the doubly excited autoionizing states) as well as the total probabilities for single and double ionization. The correct treatment of electronic correlation in the framework of the sudden approximation is shown to modify the P_K value (the probability that an atomic K vacancy is created) by more than 2%.

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Nuclear transmutations (i.e., change in the nuclear charge) induced by nuclear reactions or radioactivity are often accompanied by a redistribution of the electrons around the final transmuted nucleus. Electrons originally in the ground state of the target atom can be excited either in the bound spectrum or to the continuum of energy. Therefore, calculations of the population distribution of the atomic states of the daughter atom require a complete description of both the bound spectrum and the continuum of energy.

We propose here a numerical approach which makes use of B-spline basis sets to describe the relevant atomic states [1]. The B-spline functions are L^2 integrable polynomials which are defined on intervals. Their ''local'' character is in contrast to, for example, Slater or Gaussian functions which are ''globally'' defined. One of the essential properties of the B-spline basis sets is their ''effective'' completeness which allows the entire spectrum of an atom, including the continuum states, to be replaced by a pseudospectrum containing only a finite number of states. This pseudospectrum is constructed in a way that the low lying states represent well the low lying bound states of the real spectrum with the remaining pseudostates representing the remaining bound and continuum spectrum.

First, we have studied the electronic rearrangement induced by the β decay of ^{6}He$^+$. This one-electron system has been chosen so that the accuracy of our approach may be assessed by comparing our numerical B-spline results with analytical values for the electronic transition probabilities. However, the main purpose of this work is to treat the polyelectronic system

$$ {}^{6}_{2}\mathrm{He}_4 \rightarrow ({}^{6}_{3}\mathrm{Li}_3^{+})^* + e^- + \bar{\nu}_e , \tag{1}$$

where $\bar{\nu}_e$ is the electron antineutrino. We have calculated within the framework of the sudden approximation [2] (since the velocity of most β^- electrons are quasirelativistic) the population of the bound and continuum ^{1}S states of Li$^+$ populated during the β decay of ^{6}He. We obtained in one diagonalization an accurate representation of a number of bound Rydberg states, of doubly excited states and of the continuum.

In our approach, the one-electron radial Schrödinger equation for a hydrogenic system is solved in a cavity of radius R using the Rayleigh-Ritz-Galerkin scheme [3]. The mono-electronic radial distribution is expressed as a linear combination

$$P_{n\ell}(r) = \sum c_i B_{i,k}(r), \tag{2}$$

where the B splines $\{B_{i,k}(r)\}$ are positive piecewise polynomials of order k. The radial interval $[0,R]$ is divided into segments $[t_i, t_{i+1}]$ $(t_{i+1} \geqslant t_i)$ by a ''knot sequence'' $[t_i]$. The B splines are defined on this knot sequence by recursion relations. More information on the properties of the B splines can be found in the book by de Boor [4]. In this work, 25 B splines of order 7 and a cavity radius of 100.0 a.u. have been used. These parameters have been chosen so that accurate results are obtained with a minimum number of basis functions for the one and two-electron systems considered here. Because the majority of the states involved in the transitions are low lying bound states and, in the case of two-electron systems, the lowest doubly excited states of the spectrum, an exponential grid has been used which allows for a larger number of B splines near the origin where the wave function varies rapidly.

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TABLE I. Transition probabilities to various $^{6}\mathrm{Li}^{2+}$ states induced by the β decay of the $^{6}\mathrm{He}^{+}$ ion. Both B-spline results and analytical values are given in %.

	$\lvert T_{fi}^{(0)}\rvert^2$	
Final $^{6}\mathrm{Li}^{2+}$ state	B spline	Analytical
1s	88.47360	88.47360
2s	7.67360	7.67360
3s	0.86708	0.86708
4s	0.28190	0.28190
5s	0.12909	0.12908
6s	0.07046	0.07045
7s	0.04285	0.04285
8s	0.02800	0.02808
Remaining bound states	0.10297	0.09523[a]
Continuum	2.33643	2.33

[a] Summation up to $n=500$.

The two-electron wave functions are obtained by a CI (configurations interaction) method using basis of configurations built on the monoelectronic orbitals [5]. Because the sudden approximation without recoil has been used in this work, only the ^{1}S states of Li^{+} can be populated after the change in the nuclear charge. The configurations included in our calculations are ns^2, $nsn's$, np^2, $npn'p$, nd^2, $ndn'd$, nf^2, and $nfn'f$. This combination takes into account the major effects of electronic correlation. The same configurations are included in the calculation of the ground state of He.

In the framework of the sudden approximation, if we neglect the effect of the recoil of the daughter nucleus, the transition probability to a final atomic state is simply given by

$$|T_{fi}^{0}|^2=(\Psi_f|\Psi_i)^2, \tag{3}$$

where Ψ_i corresponds to the wave function of the initial state with nuclear charge Z and Ψ_f to the wave function of the transmuted ion with nuclear charge Z' (with $Z'=Z+1$ for β decay). The orthonormality constraint between the final state wave functions implies that the sum over all the transitions involving the same initial state is one. A major advantage of the B-spline approach is to preserve the orthogonality between the final wave functions since they all come from the same diagonalization.

For the β decay of $^{6}\mathrm{He}^{+}$, the initial state is the 1s ground state of the helium ion while the final states appearing in Eq. (3) belong to the ns-εs spectrum of Li^{2+}. The ^{2}S B-spline Rydberg series of Li^{2+} can be divided in three parts: 8 eigenvalues correspond to the lowest lying bound states, 6 eigenvalues represent pseudobound states (i.e., states which have an energy less than zero but which are not ''real'' states), and 11 states with positive energy which are pseudocontinuum states. The transition probabilities are calculated numerically from Eq. (3) using Gauss-Legendre quadrature and are compared with the analytical values in Table I for the lowest ns states. The summation over all the pseudocontinuum states gives 2.33% for the ionization probability or shake-off mechanism while the excitation in the bound spectrum, i.e., the sum over all the probabilities of the ''real'' and pseudobound states, is 97.6696%. This number can be compared with the analytical sum over the 500 lowest bound states which is 97.6619% and thus demonstrating the effectiveness of the B-spline basis set.

TABLE II. Eigenvalues in a.u. and excitation energies in cm^{-1} for the $1sn\ell$ ^{1}S states in Li^{+}. The total energies obtained in this work are compared to the results of Drake [19] for the ground state and of Kono and Hattori [20] for the excited states while the differences of energy are compared with Bashkin and Stoner [21].

State	B spline	Hylleraas	B spline	Expt.
$1s^2$ ^{1}S	−7.2793492	−7.2799135	0	0
$1s2s$ ^{1}S	−5.0408201	−5.0408767	491262	491334.6
$1s3s$ ^{1}S	−4.7337397	−4.7337556	558653	558777.88
$1s4s$ ^{1}S	−4.6297767	−4.6297832	581464	581596.77
$1s5s$ ^{1}S	−4.5824240	−4.5824274	591860	591989.55
$1s6s$ ^{1}S	−4.5569496		597451	597580.53
$1s7s$ ^{1}S	−4.5416882		600800	600930
$1s8s$ ^{1}S	−4.5318274		602964	
$2s^2$ ^{1}S	−1.904924	−1.905845[a]		
$2p^2$ ^{1}S	−1.628787	−1.630439[a]		

[a] Reference [7].

To assess the accuracy of our B-spline wave functions for two electron systems, we now look at the total energies of the discrete states of He and Li^{+}. Using the B-spline basis described above, the total energy of the ground state of the He atom is −2.903 309 69 a.u., in good agreement with the result of Frankowski and Pekeris [8], −2.903 724 377 a.u., obtained using Hylleraas type functions. This last calculation takes into account electron correlation effects of all ℓ values while the B-spline calculation only includes electron angular momentum up to $\ell=3$. For comparison, the HF (Hartree-Fock) value for the He ground state is −2.861 680 0 a.u.

The total energies of the lowest members of the Li^{+} ^{1}S Rydberg series obtained using the same B-spline basis set are shown in Table II. The B-spline results are compared with the available Hylleraas values for the five lowest ^{1}S states. In one diagonalization, the B-spline approach gives accurate results for the eight lowest members of the ^{1}S series. The excitation energies of these states are compared with the experimental values in Table II. Also given are the total energies of the two lowest ^{1}S doubly excited states, $2s^2$ ^{1}S and $2p^2$ ^{1}S, located above the first ionization threshold. It has been shown [6] that for this type of state the contribution of electronic correlation is very large and that only the inclusion of electrons with high angular momentum can insure an accurate description of their spectral properties. In this respect, the agreement between our B-spline results and the complex-coordinate values of Ho [7] obtained using Hylleraas basis sets is satisfactory.

Having discussed the accuracy of our wave functions, we now present the transition probabilities to all the final Li^{+} states, calculated using Eq. (3). The transition probabilities to the discrete Li^{+} states larger than 0.1% are given in Table III. Comparing these results with the $^{6}\mathrm{He}^{+}$ probabilities given in Table I, it is clear that the probability that the atom remains in the ground state is smaller for neutral He than for He^{+}, while the excitation process to the $1s2s$ ^{1}S Li^{+} state is larger than the excitation probability to 2s state of Li^{2+}. The

TABLE III. Transition probabilities (in %) to the Li^+ states induced by the β decay of ^{6}He in the sudden approximation without recoil.

Final $^6Li^+$ state	$\lvert T_{fi}^{(0)}\rvert^2$ B splines	 Winther [2]
$1s^2\ ^1S$	70.85	67.0
$1s2s\ ^1S$	14.94	16.6
$1s3s\ ^1S$	1.86	2.7
$1s4s\ ^1S$	0.62	0.8
$1s5s\ ^1S$	0.29	
$1s6s\ ^1S$	0.16	
$1s7s\ ^1S$	0.10	
$2s^2\ ^1S$	1.56	
$2p^2\ ^1S$	0.18	
$2s3s\ ^1S$	0.23	

transition probability to the $1s3s\ ^1S$ of Li^+ is larger than the transition probability to the $3s$ state in any one electron system including tritium. This probability decreases much more slowly with increasing n than for the one-electron case.

For two electron systems, excitation to autoionizing states is also possible. Although excitation to the $2s^2\ ^1S$ state is still important, the probabilities decrease rapidly for the $2sns\ ^1S$ and $2pnp\ ^1S$ series with only $2p^2$ and $2s3s$ having probabilities greater than 0.1%.

We compare in Table III our results with the pioneering work of Winther [2]. In his work, the wave functions used for the ground states of He and Li^+ as well as the lowest excited Li^+ state were restricted Hylleraas expansions while Hartree wave functions were used for the other excited Li^+ states. Note that contrary to the B-spline wave functions, the Li^+ wave functions used by Winther are not orthogonal which implies that the sum over the transition probabilities to all the Li^+ states is not one. The difference between the two sets of values are important especially for the probability that the atom remains in the ground state. To verify our result, we have performed a MCHF (multiconfiguration Hartree Fock) calculation for both the He and Li^+ ground states. This approach is based on a numerical solution of the MCHF equations [9]. The wave functions used were built as linear combinations of the configurations $\{1s^2,2s^2,2p^2,3s^2,3p^2,3d^2,4s^2,4p^2,4d^2,4f^2\}$ and due to the property of the reduced form of the pair-correlation function [10] must be very similar to the B-spline wave functions. The probability obtained using this approach is 70.84% in very good agreement with the B-spline value. We have also verified, using the same approach, that the inclusion of higher ℓ values in the MCHF expansion does not influence significantly this probability. We note that the influence of electronic correlation is important in the evaluation of the probabilities. For example, the HF value for the probability that the atom remains in the ground state is 73.1%, i.e., more than two percent larger than the correlated value.

TABLE IV. Total transition probabilities (in %) for the population of different electronic states induced by the β decay of ^{6}He.

Final $^6Li^+$ state	Total probability
Bound states	89.09
Autoionizing states	2.97
Ionization of one electron	7.47
Ionization of two electrons	0.32

Our method allows the calculation of not only the transition probabilities to discrete states but also the ionization probability of one or two electrons. The total probabilities for these different mechanisms are given in Table IV. All the ionization-excitation probabilities to the different $n\ell$ limits ($n=2-\infty$ and $\ell=0-4$) are included in the total probability to ionize one electron. Similarly, the total excitation probability to autoionizing states contains the transition probabilities to all the autoionization states ($2\ell n\ell'$, $3\ell n\ell'$, $4\ell n\ell'$, etc.). Individual probabilities of less than 10^{-5} have been neglected in the summations.

The single ionization probability is 7.47% while double ionization accounts only for 0.32%. Winther obtained a total probability of 89.5% to populate discrete states. This was determined by adding the values shown in Table III and by extrapolating the contributions of the remaining discrete states. This result gives an ionization probability (single and double ionization as well as the contribution of doubly excited states) of (10.5±1.5)% to be compared with our result of 10.8%. Using a radioactive recoil spectrometry experiment, Carlson *et al.* have [11] measured that the single ionization probability is (10.4±0.2)% and the B-spline value of 10.4% agrees very well with this result. In the same experiment, the double ionization probability has been found to be much less likely (0.042±0.007)% than our estimation of 0.3%.

Finally, we consider the quantity P_K, the probability per nuclear disintegration that an atomic K vacancy (a hole in the $1s^2$ shell) is created [12]. In the sudden approximation this quantity is simply given by $1-[\langle\Psi_f(1s^2\ ^1S)|\Psi_i(1s^2\ ^1S)\rangle]^2$. If electronic correlation effects are not taken into account this expression reduces to $1-(1s_f|1s_i)^4$, the $1s$ radial distributions being optimized in for example a Hartree-Fock procedure. This approach has been used by Carlson *et al.* [13] who predicted a P_K value of 26.9% for the β decay of ^{6}He. However, the introduction of electronic correlation in our approach increases significantly the probability to 29.15%. Law and Campbell [12] obtained a P_K value of 27.61% for the β decay of ^{6}He. Unfortunately, their results suffer from an error discovered by Isozumi *et al.* [14] and clearly explained by Cooper and Åberg [15]. The new value obtained for ^{6}He by Isozumi *et al.* is 22.91%. However, we would like to stress again the fact that our wave functions take into account the correlation effects, which have been neglected in all the previous treatments, and are orthonormal. With respect to the latter, they elude the criticism formulated by Law and Suzuki [16] concerning the wave functions used in the previous studies [12–14].

However, it seems useful to clarify the sudden approximation we use. It is based on the assumption that the β electron crosses the electronic distribution around the daughter nucleus instantaneously producing a sudden change of the nuclear charge. It differs radically from the "one step model" of Cooper and Åberg [15] and from the "one active electron model" of Law and Campbell [12] which take into account the effect of the Pauli principle for the β particle and the ejected atomic electron. However, in the case of He, our approximation is justified by the fact that the average energy of a β electron is several thousands time larger than the binding energy of a K electron. One verifies with the formula discussed by Cooper and Åberg that the exchange term will be negligible in this case. We are aware of the fact that the sudden approximation is not well adapted to the study of numerous β radioactivities treated by [16] for elements with values of Z between 17 and 83; in these cases the maximum β energy is not as large as in ^{6}He and moreover the K-binding energies are markedly larger.

To conclude, we have demonstrated a new B-spline approach, which includes electronic correlation effects, to calculate the electronic rearrangement induced by β decay. These effects have been shown to be important in, for instance, determining accurately a quantity like the probability that an atomic K vacancy is created, P_K. Our method is not restricted to the use of the sudden approximation and work is in progress to include the main corrections to this approximation, for example in the case of nuclear reactions. The effect of the recoil of the daughter nucleus is small for the β decay of ^{6}He; the maximum energy for this nucleus occurs at 3.5 MeV [17] so that the β particle can be considered to be quasirelativistic. However, the population of states with symmetries $^1P, {}^1D, \ldots$ resulting from the recoil effect must be taken into account in the interpretation of the experimental data related to nuclear reactions like the resonant α-α scattering [18]

$$^4\mathrm{He}^{2+} + {}^4\mathrm{He} \rightarrow ({}^8\mathrm{Be}^{2+})^*. \tag{4}$$

We plan to apply our approach to this process in the future.

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