

TABLE I: Population probabilities P_n of the 1S bound states of helium after the β decay of a T^- anion. Also given are the corresponding energies E_n (in atomic units) obtained in the present work.

n	E_n (this work) ^a	$P_n(\%)$ (this work)	$P_n(\%)$ (Ref. 17)	$P_n(\%)$ (Ref. 18)
1	-2.9034572	22.98998	22.993764	19.147
2	-2.1459527	46.86960	46.867404	21.149
3	-2.0612659	0.01320	0.135	0.27
4	-2.0335841	0.18363	0.21	0.143
5	-2.0211749	0.09220	—	0.07
6	-2.0145604	0.05262	—	0.039
7	-2.0106235	0.03275	—	0.024
8	-2.0080909	0.02175	—	0.016
9	-2.0063679	0.01522	—	0.011
10	-2.0051407	0.01111	—	0.008
11	-2.0042355	0.00848	—	—
12	-2.0035507	0.00666	—	—
13	-2.0030205	0.00513	—	—
14	-2.0025951	0.00469	—	—
15	-2.0022570	0.00273	—	—
$\sum P_n$		70.30975	70.206168	40.877

^aThe bold digits agree with the results in Ref. 25.

angle θ can in principle be chosen arbitrarily within $0^\circ \leq \theta \leq 45^\circ$. In the limit of an infinite basis all observables calculated with the aid of complex scaling should become independent of θ . Since only finite basis sets can be applied in practice, only approximate eigenstates can be obtained that may depend on θ . The angle θ can thus be understood as a variational parameter that modifies the adopted basis as can be seen from the inverse relation between basis-set exponents and the scaling angle discussed, e. g., in [29]. A diagonalization of the Hamiltonian (8) in the basis described by the Eqs. (4) and (5) yields the complex-scaled energies $E_j(\theta)$ and wavefunctions $\Psi_j(\theta)$ where the latter are still defined by Eq. (6), but with complex coefficients $c_{jk}(\theta)$.

With the aid of the complex-scaled energies and wavefunctions the transition-probability density into the electronic continuum can be extracted from the complex-scaled resolvent according to [9]

$$P(E, \theta) = \frac{1}{\pi} \text{Im} \left\{ \sum_k \frac{\langle \Psi_i^{T^-}(\theta^*) | \Psi_k^{\text{He}}(\theta) \rangle \langle \Psi_k^{\text{He}}(\theta^*) | \Psi_i^{T^-}(\theta) \rangle}{E_k^{\text{He}}(\theta) - E} \right\}. \quad (9)$$

The $\langle \Psi(\theta^*) |$ is the biorthonormal eigenstate to $|\Psi(\theta)\rangle$. It is obtained from the latter by a transposition and complex conjugation of the angular part, while the radial part is only transposed but not complex conjugated. The sum over k includes all complex-scaled eigenstates and eigenvalues calculated by solving the generalized complex symmetric, but non-hermitian eigenvalue problem. As dis-

cussed above in the limit of exact eigenstates the density $P(E, \theta)$ becomes independent of the complex-scaling parameter θ . A variation of θ for approximate eigenstates provides the possibility to determine an optimal θ_{opt} with highest stability. The best approximation of $P(E, \theta)$ is then obtained according to

$$\left. \frac{\partial P(E, \theta)}{\partial \theta} \right|_{\theta_{\text{opt}}} = \min. \rightarrow P(E) := P(E, \theta_{\text{opt}}). \quad (10)$$

Furthermore, the θ dependence of the spectra gives an indication for the convergence of the results.

III. RESULTS

In Table I the calculated transition probabilities for 15 1S bound states of He are listed. The results reveal that almost every second T^- decay will end in the first excited state of He. The next probable final state is the He ground state with nearly 23%. With a summed probability of 0.45% the higher excited He states are rarely populated after β decay of T^- . The sum over all calculated bound states yields 70.3%. The summation over all calculated states (discrete and discretized continuum states) yields the expected value of 100.00%, since the same basis is used for initial and all final states, but indicates the proper numerical implementation. The excellent agreement of the energy eigenvalues at the order of $\mu\text{hartree}$ with the very accurate data in [25] assures on the other hand the high quality of the basis set adopted in the present work and its ability to describe many states simultaneously with high precision. A closer view on the energies shows that the degree of accuracy of the present results follows the expected trends. First, the accuracy increases with n , since the importance of correlation decreases, if the state becomes more asymmetric and the two electrons have smaller spatial overlap. For even higher values of n the states become increasingly diffuse and thus it is very difficult to describe them properly without running into numerically caused linear dependencies.

A comparison to the final-state probabilities reported by Frolov [17] and Harston and Pyper [18] is also given in Table I. Especially for the highly populated ground and first excited states the results of this work confirm the expectedly very accurate results of Frolov [17] that were obtained with explicitly correlated basis functions. The agreement for the third excited state ($n = 4$) is, however, less good, and for the second excited state ($n = 3$) there is even an order of magnitude difference. All attempts to improve the basis set for this state failed to yield a better agreement. This could be an indication for a typographical error (a missing zero after the decimal point) in [17].

The comparison with the results in [18] that were obtained with a relativistic MCDF (multi-configuration Dirac-Fock) method shows on the other hand pronounced