PHYSICAL REVIEW A VOLUME 49, NUMBER 6 JUNE 1994

Calculation of doubly excited states of helium with a finite discrete spectrum

E. Lindroth*

Department of Physics, Chalmers University of Technology and the University of Gothenburg, S-412 96 Göteborg, Sweden

(Received 21 January 1994)

Doubly excited states in helium are calculated with many-body perturbation theory to all orders in the electron-electron interaction. A finite and numerical basis set, rotated out into the complex plane, is used. Results, for energies and widths, are presented for states with electrons in the $n = 2$ and $n = 3$ states. The possibility of an accuracy of a few parts in 10^6 is demonstrated. The method is equally applicable to the study of doubly excited states of many-electron systems and the extension to the corresponding relativistic procedure is straightforward.

PACS number(s): 31.20.Di, 31.50.+w, 31.20.Tz, 32.70.Jz

I. INTRODUCTION

The doubly excited states of helium have been the target of a number of theoretical approaches. The importance of electron-electron correlation in these states makes them interesting test cases for accurate theoretical methods. The energy released when one electron falls down into an available n shell below is enough to send another electron out from the same, or higher, n shell into the continuum. Thus most of these states are autoionizing. The width due to the presence of this process is of pure two-electron origin and is supposed to be especially sensitive to the quality of the wave functions.

Among the methods applied to these systems are the Feshbach projection formalism, which has been used by Bhatia and Temkin [1,2], and the close-coupling approximation employed by Oza [3]. The method of complex rotation, which makes bound state methods applicable to autoionizing states, has been used by Ho and co-workers [4–14] and by Chung and Davis [15]. Recently the multiconfigurational Hartree-Fock method has been extended to autoionizing states by Froese-Fischer and Idrees [16] and Tang *et al.* [17] have used a hyperspherical close-coupling method based on a numerical basis set.

Alternative classification schemes for doubly excited states have been discussed and developed by Herrick and Sinanoglu [18], Fano [19], Lin [20], and Rau [21]. A review can be found in Ref. [19].

In this work we show how the methods which use finite numerical basis sets [22–24] to produce accurate results for bound states can be extended to autoionizing states by the use of complex rotation. The change needed is not very extensive and can be introduced in the nonrelativistic as well as in the relativistic schemes.

Here nonrelativistic calculations are performed for doubly excited states in helium with the electrons in the $n = 2$ and $n = 3$ shells. In Sec. II the method is briefly described and the results are discussed in Secs. III and IV. Comparison is done with some accurate calculations and with experiments, when available.

II. THEORY

This calculation uses complex rotation combined with the method developed by Salomonson and Öster [22]. As described in [22] the atom is placed in a spherical box and inside the box a discrete radial grid is used. Diagonalization of a discretized one-particle Hamiltonian gives a discrete basis set, complete on the grid chosen. The basis set is then used to construct correlated wave functions to all orders in the perturbation expansion of the residual electron-electron interaction. The method has been applied to several many-electron systems, both in its nonrelativistic [25–28] and its relativistic [23,29–34] version. The method is able to provide accurate results as demonstrated, e.g., for the ground state of helium [22], where the calculated total energy $-2.903\,724\,39$ a.u. compares well with the "exact result" $-2.903\,724\,377\,034\,105(28)$ a.u. [35].

When perturbation theory is applied to autoionizing states it is obvious that the use of a discrete basis set will cause problems close to the poles in the energy denominator. A complex scaling of the radial coordinates can, however, solve this problem. The method of complex rotation has a rather long history [36–38] and has been used together with several approaches to atomic calculations in order to be able to use these also on autoionizing states. Ho and co-workers have combined complex rotation with the use of Hylleraas functions [38,4–14]; Chung and Davis have combined it with configuration interaction (CI) [15].

Very accurate results can be produced with Hylleraas wave functions, for autoionizing states as well as for states below the first ionization threshold. However, this method is difficult to extend to systems with more than two or three electrons. In contrast the method presented here, which uses a multipole expansion of the electron-electron interaction, is applicable to many electron atoms in general. Provided enough terms are kept in the multipole expansion, it is also possible to get agreement with

---

*Electronic address: f3aeva@fy.chalmers.se

1050-2947/94/49(6)/4473(8)/$06.00

the Hylleraas calculations to at least six digits, as will be demonstrated below.

The underlying theory of complex rotation has been discussed in many articles [36,5,37] and only a brief account of how it is applied together with many-body perturbation theory and a finite discrete basis set will be given here.

A. Complex rotation

The radial coordinates are scaled with a complex constant $r \rightarrow re^{i\theta}$. The radial one-particle Schrödinger equation then transforms to

$$\left\{ -\frac{\hbar^2}{2m}\frac{d^2}{dr^2}e^{-i2\theta} + \frac{\hbar^2}{2m}\frac{\ell(\ell+1)}{r^2}e^{-i2\theta} + eV(re^{i\theta}) \right\} P(re^{i\theta}) = \epsilon P(re^{i\theta}). \quad (1)$$

In [22] it is described how the unrotated Schrödinger equation can be discretized on a lattice to yield a real symmetric eigenvalue problem. With the complex scaling we will instead have to find the eigenvalues and the eigenstates of a complex symmetric (i.e., non-Hermitian) matrix. As in the unrotated case a choice of an N-point lattice will give N orthogonal basis set orbitals. Since the atom is put in a box, only the basis set orbitals with negative eigenvalue, those which are confined in space, will correspond to physical states. The eigenvalues of these physical states will not be affected by the complex scaling. This is expected since these states are vanishing outside the box and the matrix equation represents well the original differential equation (1), which eigenvalues should remain the same after a variable transformation. The positive eigenvalues, however, which eigenvectors constitute a pseudocontinuum, will now be complex numbers.

When the perturbation expansion is made with this complex basis set the imaginary parts of the pseudocontinuum energies will ensure that all terms are finite. The summation over intermediate states corresponds to an integration following a contour in the complex plane to avoid the poles which are situated at the real axis. Provided the rotation is large enough to achieve imaginary parts which are not too small when the real part of the energy denominators goes through zero, the numerical procedure is stable and the results will not be affected by the specific rotation angle chosen. Typically only relatively small rotation angles, $\theta \approx 10°$, are needed to calculate autoionizing states with both electrons in the $n = 2$ shell. The result is then checked to be stable up to $\theta \approx 40°$. When both electrons are in the $n = 3$ shell, however, the system can autoionize by emitting a less energetic electron and a larger rotation angle is needed. Generally, a rotation angle of $\theta \approx 35°$ is used in the calculations presented here.

The correlated energies are calculated as described in Ref. [22], but they will now be complex numbers. The real part gives the position of the resonance and the imaginary part gives half the width.

The basis set orbitals are normalized to unity and it should be noted that the conjugate vectors $\langle \psi \mid$ are conjugated before r is replaced by $re^{i\theta}$, i.e., the radial variable is not complex conjugated. The orthogonality between the basis set orbitals is not destroyed by the rotation, although they now are eigenstates to a complex symmetric, i.e., non-Hermitian, matrix.

B. The perturbation expansion

For doubly excited states of helium it is natural to let V in Eq. (1) be the nuclear potential and treat the whole electron-electron interaction as a perturbation. Since the lowest-order description of all eigenstates which belong to the same n shell now are completely degenerate it is not possible to use a single configuration starting point for the perturbation expansion. Instead an extended model space is used [39,40,31]. The lowest-order wave function is then described by a linear combination of all the configurations, with the same parity, which are degenerate in the absence of the electron-electron interaction. The admixture of all other configurations is taken care of in the perturbation expansion, but the admixtures of the model functions are decided by diagonalization of a small matrix. A more detailed description of this procedure can be found in [31].

As is well known it is in general meaningless to classify doubly excited states of helium with specific ℓ quantum numbers since these are often not even approximately good quantum numbers. Herrick and Sinanoglu [18], Lin [20], and others have thus suggested classification schemes based on new approximately good quantum numbers. We have not employed these here, but it can be noted that the model space consisting of all degenerate configurations is equivalent to the so called doubly excited symmetry basis of Herrick and Sinanoglu [18]. Thus, for the lowest-order wave function the quantum numbers of Ref. [18] are well defined. The use of hyperspherical coordinates is more naturally connected to the new quantum numbers than the usual independent particle coordinates and has been advocated, e.g., by Lin [20] and by Lin and Macek [41]. Tang *et al.* [17] have used a numerical basis set and constructed accurate wave functions in the close-coupling approximation expressed in hyperspherical coordinates. Their results for the ($n_1 = n_2 = 2$) and the ($n_1 = 2, n_2 = 3$) states agree well with the results presented here for the energies, but in several cases there is a marked disagreement for the widths.

III. RESULTS

The states with both electrons in $n = 2$ have been studied with many theoretical methods. In Table I a comparison is made between this work and the complex rotation methods based on Hylleraas wave functions [9–11,13] and on CI [15]. The later calculation includes partial waves up to $\ell_{max} = 3$ for the ^1S state and up to $\ell_{max} = 4$ for the ^1P state. This is probably the source of the small deviation from the results presented here, which includes $\ell_{max} = 11$ or $\ell_{max} = 10$ and are extrapolated from there. The convergence pattern when higher ℓ values are included is seen in Table II for the $(2s2p)^{1,3}P$ states and in Table III for the even-parity states. As is usually found the triplet states converge faster than the singlet states. After the ℓ sum is extrapolated the results agree within a few units in the sixth decimal with the results by Ho and Bhatia [9–11,13], where Hylleraas-type wave functions were employed and thus no expansion in partial waves is done. Oza [3] uses a very different method based on scattering theory. The widths are obtained from the calculated phase shifts and he uses an algebraic variational method. Also here the minor deviation is probably due to the smaller number $\ell_{max} = 3$ of partial waves included.

For the nonautoionizing state $(2p^2)^3P$ some very accurate calculations exist [42–44]. Here the $(2p^2)^3P$ state is calculated together with the autoionizing states. The width of this state then has to be zero by numerical means. It is indeed approaching zero and with the numerical setup used here a spurious width of only 10^{-14} a.u. is obtained, which reflects the numerical accuracy.

For the states with one electron in $n = 2$ and one electron in $n = 3$ accurate calculations exist by Ho and Bhatia [9–11,13] and by Oza [3]. The agreement between the methods is generally very good, as can be seen in Table IV. For the very narrow width of the third $^3P^o$ there is, however, a slight disagreement. The result obtained here is 25% larger than the result obtained by Ho and Bhatia. Although there is a state of the same symmetry rather close in energy—a $(2\ell 4\ell')^3P^o$ state is $< 6 \times 10^{-3}$ a.u. above [3]—which possibly could destroy the convergence of the state in question, see below, there is no sign of such problems. The width seems well converged and in some other cases we find results in good agreement with Ho and Bhatia in spite of an even closer level of the same symmetry. For example, $< 3\times 10^{-3}$ a.u. above the highest $^1S^e$ state in Table IV there is another level of the same symmetry. The second $(3\ell 3\ell')^1P^o$ state in Table V is another example, which is discussed below.

Also for the states with both electrons in the $n = 3$ shell calculations have been performed by Ho and Bhatia [9,11–14] and by Ho and Callaway [8] and the results are listed in Table V. In most cases the agreement is rather good. However, the width of the $^3F^o$ state, which Ref. [8] finds to be $< 1 \times 10^{-6}$ Ry, is here determined to be 3.13×10^{-5} a.u., i.e., 6.26×10^{-5} Ry. Although the perturbation approach used here has problems with a small number of states, that does not apply to this state. The problems, discussed below, arise when two physical states are very close to each other and they manifest themselves by, usually slowly, diverging energy values. The $^3F^o$ state is far away from any other state of the same symmetry and the width is converged to at least eight digits.

A few states with the same symmetry are extremely close in energy. For example, the highest $(2\ell 3\ell')^1P^o$ state is only 6×10^{-4} a.u. below the lowest $(2\ell 4\ell')^1P^o$ state [10]. The highest $(2\ell 3\ell')^1P^o$ state then converges slowly and the prediction of the narrow width is rather unstable. That this width is very sensitive to the quality of the

TABLE I. Energies and widths of the $n_1 = n_2 = 2$ states in helium obtained with different methods. The results are given in atomic units (a.u.) for energy. 1 a.u. $= 2$ Ry $= 27.211\,396(1 - \frac{m}{M})$ eV. The $^3P^e$ state is nonautoionizing due to symmetry reasons.

	Present[a]		Ho and Bhatia[b]		Oza[c]		Chung and Davis[d]		Bhatia[e]
	E	Γ	E	Γ	E	Γ	E	Γ	E
$^1S^e$ (1)	-0.777868	0.004541	-0.777868	0.00453	-0.7778	0.00458	-0.777858	0.0045707	
$^1S^e$ (2)	-0.621926	0.000216	-0.6219275	0.0002156	-0.620516	0.000231			
$^3P^e$	-0.710500								-0.7105002
$^1D^e$	-0.701946	0.002362	-0.7019457	0.0023622	-0.701655	0.00241			
$^3P^o$	-0.760492	0.000299	-0.760492388	0.000298862	-0.7604512	0.000301			
$^1P^o$	-0.693135	0.001373	-0.6931349	0.0013733	-0.6928	0.00133	-0.693024	0.0013731	

[a] Partial waves included up to $\ell_{max} = 11$ for the odd-parity states and, extrapolated from there, $\ell_{max} = 10$ included for the even-parity states.

[b] Hylleraas wave functions and complex rotation $^1S^e$, Ref. [9]; $^1D^e$, Ref. [11]; $^1P^o$, Ref. [10]; and $^3P^o$, Ref. [13].

[c] Close-coupling method, $\ell_{max} = 3$, Ref. [3].

[d] Configuration interaction and complex rotation, $\ell_{max} = 3$ for ^1S and $\ell_{max} = 4$ for ^1P, Ref. [15].

[e] Reference [42], where the full result $-0.710\,500\,152\,07$ a.u. is given.

TABLE II. Convergence of the energies and widths of the $(2s2p)^{1,3}P$ states in helium when the number of included partial waves is increased. The results are given in atomic units (a.u.) for energy. 1 a.u. = 2 Ry = 27.211 396$(1 - \frac{m}{M})$ eV.

	$(2s2p)^1P$		$(2s2p)^3P$	
	E	Γ	E	Γ
$\ell_{max} = 4$	-0.6929940	0.00137247	-0.7604845	0.00029882
$\ell_{max} = 8$	-0.6931160	0.00137308	-0.7604921	0.00029885
$\ell_{max} = 9$	-0.6931215	0.00137311	-0.7604922	0.00029885
$\ell_{max} = 10$	-0.6931251	0.00137314	-0.7604923	0.00029885
$\ell_{max} = 11$	-0.6931274	0.00137315	-0.7604923	0.00029885
extrapolated	-0.693135	0.001373	-0.760492	0.000299

TABLE III. Convergence of the energies and widths of the even-parity states in helium with $n_1 = n_2 = 2$ when the number of included partial waves is increased. The results are given in atomic units (a.u.) for energy. 1 a.u. = 2 Ry = 27.211 396 $(1 - \frac{m}{M})$ eV.

	^1S (1)		^1S (2)		$(2p^2)^3P$	$(2p^2)^1D$	
	E	Γ	E	Γ	E	E	Γ
$\ell_{max} = 8$	-0.7778665	0.0045422	-0.6218779	0.0002160	-0.7104992	-0.7019313	0.0023640
$\ell_{max} = 9$	-0.7778668	0.0045419	-0.6218919	0.0002160	-0.7104996	-0.7019356	0.0023636
$\ell_{max} = 10$	-0.7778670	0.0045418	-0.6219010	0.0002160	-0.7104998	-0.7019383	0.0023633
extrapolated	-0.777868	0.004541	-0.621926	0.000216	-0.710500	-0.701946	0.002362

TABLE IV. Energies and widths of the $n_1 = 2$ and $n_2 = 3$ states in helium obtained with different methods. The results are given in atomic units (a.u.) for energy. 1 a.u. = 2 Ry = 27.211 396$(1 - \frac{m}{M})$ eV. The $^{1,3}P^e$ states and the $^{1,3}D^o$ states are nonautoionizing due to symmetry reasons.

	Present[a]		Ho and Bhatia[b]		Oza[c]	
	E	Γ	E	Γ	E	Γ
$^1S^e$ (1)	-0.58989	1.36×10^{-3}	-0.589895	1.35×10^{-3}	-0.589865	1.38×10^{-3}
$^1S^e$ (2)	-0.54809	7.62×10^{-5}	-0.5480855	7.8×10^{-5}	-0.5478765	8.27×10^{-5}
$^3S^e$ (1)	-0.60258	6.64×10^{-6}			-0.602576765	6.42×10^{-6}
$^3S^e$ (2)	-0.55975	2.56×10^{-7}			-0.5597187	2.3×10^{-7}
$^1P^e$	-0.58025					
$^3P^e$	-0.56781					
$^1D^e$ (1)	-0.56922	5.56×10^{-4}	-0.569221	5.55×10^{-4}	-0.569115	5.7×10^{-4}
$^1D^e$ (2)	-0.55643	2.00×10^{-5}	-0.5564303	2.01×10^{-5}	-0.5563903	1.99×10^{-5}
$^3D^e$ (1)	-0.58378	3.0×10^{-8}	-0.58378427	2.86×10^{-8}	-0.58378017	3.21×10^{-8}
$^3D^e$ (2)	-0.56069	7.51×10^{-6}	-0.560687	7.5×10^{-6}	-0.5606695	7.4×10^{-6}
$^1P^o$ (1)	-0.59707	3.84×10^{-6}	-0.59707381	3.84399×10^{-6}	-0.5970725	3.89×10^{-6}
$^1P^o$ (2)	-0.56409	3.01×10^{-4}	-0.56408514	3.01057×10^{-4}	-0.56401	3.1×10^{-4}
$^1P^o$ (3)	-0.5471	$< 10^{-7}$	-0.5470927	1.507×10^{-8}		
$^3P^o$ (1)	-0.58467	8.23×10^{-5}	-0.5846723	$8.225\times^{-5}$	-0.584652	7.7×10^{-5}
$^3P^o$ (2)	-0.57903	1.88×10^{-6}	-0.57903099	1.8942×10^{-6}	-0.5790245	1.78×10^{-6}
$^3P^o$ (3)	-0.54884	1.6×10^{-8}	-0.54884435	1.27×10^{-8}	-0.54879738	1.08×10^{-8}
$^1D^o$	-0.56380					
$^3D^o$	-0.55933					
$^1F^o$	-0.55828	1.28×10^{-5}				
$^3F^o$	-0.56620	2.34×10^{-5}				

[a] Partial waves included up to $\ell_{max} = 7$ and extrapolated from there. The extrapolation does not change the triplet states to the accuracy shown here. The singlet states change not more than one unit in the last digit, with the exception of the width of the second ^1S state which change from 7.49×10^{-5} to 7.62×10^{-5} after extrapolation.

[b] Hylleraas wave functions and complex rotation ^1S, Ref. [9]; $^{1,3}D^e$, Ref. [11]; $^1P^o$, Ref. [10]; and $^3P^o$, Ref. [13].

[c] Close-coupling method, $\ell_{max} = 3$, Ref. [3].

wave function has been demonstrated by Ho [10]. His result, 1.507×10^{-8} a.u., was obtained with Hylleraas wave functions with 1140 terms. With 969 terms a rather different result, 4.403×10^{-8} a.u., was obtained. In Table IV the result for the energy position of the highest $^1P^o$ state is given with fewer digits due to these complications and the width is only indicated. A similar situation exists for the highest $(3\ell3\ell)^1S$ state, which is 1×10^{-3} a.u. below the lowest $(3\ell5\ell)^1S$ state. In addition two $(3\ell4\ell)^1S$ states lie below the highest $(3\ell3\ell)^1S$ state [9]. This situation cannot be treated without special considerations and thus this level is not calculated here. Also the second $(3\ell3\ell')^1P^o$ state is very close, and above, the lowest $(4\ell3\ell')^1P^o$ state. The difference is only 2×10^{-3} a.u. [8]. As a consequence of this the width is less well converged than for most other states, although the result in Table V is accurate to the number of digits shown. This result also agree well with the result by Ho and Callaway.

IV. COMPARISON WITH EXPERIMENTS

A. Photoabsorption experiments

The $^1P^o$ states can be observed in photoabsorption experiments. Since the classical measurement by Madden and Codling [45,46], several measurements have been carried out [47–51]. These experiments measure the doubly excited state relative to the ground state. To obtain this energy difference we combine the results in Tables I, IV, and V for the excited states with the vlaue $-2.903\,783\,8$ a.u. for the ground state. The latter value is the sum of the helium ionization potential, including mass polarization and relativistic and radiative effects, calculated by Drake [52], $-0.903\,693\,7$ a.u., and the relativistic He^+ energy, $-2.000\,106\,5$ a.u., corrected for radiative effects [53], $0.000\,016\,4$ a.u. The result in eV is obtained after multiplication with $27.207\,665$, which is the conversion factor corrected for reduced mass. The present results for the excited states are nonrelativistic and without mass polarization, but the corrections due to these effects have been calculated for the $(2s2p)^1P$ state by Chung and Davis [54]. Their result was -0.26×10^{-4} a.u., which decreases the theoretical value on the first row of Table VI with 0.0007 eV, as indicated on the second row. Corrections of this size are, however, beyond the experimental uncertainty.

As can be seen in Table VI the theoretical result for the energy position of the $(2s2p)^1P$ state agrees rather well with the experiment by Morgan and Ederer [48], but according to the other measurements the theoretical result is only just covered by the error bars. There is also a recent measurement from the Berliner Electronenspeicherring-Gesellschaft für Synchrotronstrahlung facility [51], which seems to support the result by Morgan and Ederer for the energy position, but this experiment claims a width of 0.0423 ± 0.0023 eV, which in not consistent with theory and hardly with the

TABLE V. Energies and widths of $n_1 = n_2 = 3$ states in helium obtained with different methods. The results are given in atomic units (a.u.) for energy. 1 a.u. = 2 Ry = $27.211\,396\,(1-\frac{m}{M})$ eV.

	Present[a]		Ho *et al.*[b]	
	E	Γ	E	Γ
$^1S^e$ (1)	-0.35354	3.01×10^{-3}	-0.353537	3.004×10^{-3}
$^1S^e$ (2)	-0.31745	6.67×10^{-3}	-0.317455	6.67×10^{-3}
$^1S^e$ (3)			-0.2573716	2.09×10^{-5}
$^3P^e$ (1)	-0.33609	4.49×10^{-3}	-0.3360879	4.4887×10^{-3}
$^3P^e$ (2)	-0.29115	7.41×10^{-5}	-0.29115823	7.40×10^{-5}
$^1D^e$ (1)	-0.34317	5.16×10^{-3}	-0.343173	5.155×10^{-3}
$^1D^e$ (2)	-0.31554	4.29×10^{-3}	-0.31553	4.305×10^{-3}
$^1D^e$ (3)	-0.29009	1.26×10^{-3}	-0.290092	1.261×10^{-3}
$^3D^e$	-0.32533	7.24×10^{-4}	-0.325331	7.25×10^{-4}
$^3F^e$	-0.31072	1.98×10^{-3}	-0.310725	2.08×10^{-3}
$^1G^e$	-0.30712	6.63×10^{-3}	-0.30705	6.70×10^{-3}
$^1P^o$ (1)	-0.33563	7.02×10^{-3}	-0.3356259	7.023×10^{-3}
$^1P^o$ (2)	-0.28283	1.45×10^{-3}	-0.28282897	1.4621×10^{-3}
$^3P^o$ (1)	-0.35038	2.99×10^{-3}	-0.3503777	2.9866×10^{-3}
$^3P^o$ (2)	-0.30938	1.12×10^{-3}	-0.30938001	1.11767×10^{-3}
$^1D^o$	-0.32823	3.21×10^{-4}	-0.32823	3.18×10^{-4}
$^3D^o$	-0.31558	2.09×10^{-3}	-0.315575	2.08×10^{-3}
$^1F^o$	-0.30424	3.25×10^{-3}	-0.304215	3.25×10^{-3}
$^3F^o$	-0.33165	3.13×10^{-5}	-0.33164	$< 0.5\times10^{-6}$

[a] For the S states partial waves included up to $\ell_{max} = 4$, otherwise partial waves included up to $\ell_{max} = 7$ and extrapolated from there. The extrapolation does not change the triplet states to the accuracy shown here and the singlet states change not more than one unit in the last digit.

[b] Hylleraas wave functions and complex rotation ^1S, Ref. [9]; $^3P^e$, Ref. [14]; $^{1,3}D^e$, Ref. [11]; $^1P^o$, Ref. [12]; and $^3P^o$, Ref. [13]. The other states are calculated with CI functions and complex rotation Ref. [8].

TABLE VI. Comparison between the present results and photoabsorption experiments for some $^1P^o$ states. The results are given in eV relative to the ground state, which has a total energy of −2.903 7838 a.u. = −79.005 18 eV including relativistic effects and mass polarization. (Refs. [52,53], see Sec. IV for details.)

	Present		Experiment			
	E	Γ	E		Γ	
$n_1 = n_2 = 2$	60.1466[a]	0.0374	60.133	±0.015	0.038	±0.004[b]
	60.146[c]		60.151	±0.010	0.038	±0.002[d]
			60.133	±0.015	0.038	±0.001[e]
$n_1 = 2,\ n_2 = 3$	63.658[g]	0.008	63.655	±0.007	0.008	±0.004[b]
			63.655	±0.010	0.0083	±0.002[d]
$n_1 = n_2 = 3$	69.874[h]	0.191	69.92	±0.03	0.132	±0.014[f]
			69.914	±0.015	0.200	±0.020[e]
			69.880	±0.022	0.180	±0.015[i]

[a] The result for the excited state is taken from Table I.

[b] Madden and Codling [45,46].

[c] Added to the result for the excited state in Table I are the corrections due to mass polarization and relativistic effects, −0.0007 eV, given in Ref. [54].

[d] Morgan and Ederer [48].

[e] Kossmann *et al.* [49].

[f] Dhez and Ederer [47].

[g] The result for the excited state is taken from Table IV, the second $^1P^o$ (2) state.

[h] The result for the excited state is taken from Table V, the first $^1P^o$ (1) state.

[i] Zubek *et al.* [50].

TABLE VII. Comparison between the present results and experiments where the doubly excited state is produced by electron impact and the observations made of the Auger electron. The results are given in eV relative to the $(2s2p)^1P^o$ state, which is used as reference in the experiments. The energy of the $(2s2p)^1P^o$ state, −0.693 135 a.u., is taken from Table I. 1 a.u. = 27.211 396 eV.

	Present		Experiment			
	E	Γ	E		Γ	
$n_1 = n_2 = 2$						
$^1S^e$ (1)	-2.306[a]	0.124	-2.31	±0.04	0.138	±0.015[b]
			-2.35	±0.03	0.138	±0.015[c]
$^1S^e$ (2)	1.938[a]	0.006	1.93	±0.03[b]		
			1.97	±0.03[c]		
$^1D^e$	-0.240[a]	0.064	-0.24	±0.03	0.072	±0.018[b]
			-0.26	±0.03	0.07	±0.018[c]
$^3P^o$	-1.833[a]	0.008	-1.83	±0.03	< 0.015[b]	
			-1.84	±0.03	~ 0.01[c]	
$n_1 = 2,\ n_2 = 3$						
$^1S^e$ (1)	2.809[d]	0.037	2.81	±0.03	0.041	±0.01[b]
$^1D^e$ (1)	3.372[d]	0.015	3.37	±0.03[b]		
$^1P^o$ (1)	3.512[d]	0.008	3.52	±0.03[b]		
$^3P^o$ (1)	2.951[d]	0.002	2.94	±0.03[b]		
			2.95	±0.03[b]		

[a] The result is taken from Table I.

[b] Hicks and Comer [55].

[c] Gelebart *et al.* [56].

[d] The results for the higher states are taken from Table IV.

other experiments either. At the level of accuracy given by the experiments the calculations listed in Table I all agree equally well with the measurements.

For the state with one electron in the $n = 2$ shell and one electron in the $n = 3$ shell the agreement between theory and experiment is good for both the position and the width. For the state with both electrons in the $n = 3$ shell there are conflicting experimental results for the width, but the theory agrees well with the more recent results [49,50]. The theoretical result for the energy position is slightly outside the experimental error bars when compared with the experimental values of Refs. [47,49], but the result by Zubek *et al.* [50] is in close agreement with theory.

B. Experiments observing the ejected electron

Only ${}^1P^o$ states can be observed in the photoabsorption experiments, but other states can be produced by electron impact. In the experiments by Hicks and Comer [55] and by Gelebart *et al.* [56] the electron ejected in the Auger process is analyzed and dependence of the resolution of the electron beam is thus avoided. In Table VII a comparison is made between theory and experiments. The experiments [55,56] used the $(2s2p)^1P^o$ state as a reference; the energy of the ejected electron was thus measured relative the energy of the electron ejected from that state. Madden and Codling's result for the ${}^1P^o$ state [46] was then used to relate the other states to the ground state. What is listed in Table VII is, however, the position relative the $(2s2p)^1P^o$ state directly, which can be compared with the energy difference given by theory. Generally the agreement for the energy positions is fair, although the calculation for the lowest ${}^1S$ state does not fall between the two experiments, which would be required if it should agree with both. The comparison for the width for the same state is just inside the error bars. The other widths agree inside rather generous error bars. To convert the calculated results to eV the conversion factor for infinite nuclear mass is used due to an effective cancellation of reduced mass and center of mass effects as explained in Ref. [1].

C. Beam-foil experiments

Some doubly excited states are not able to autoionize due to symmetry reasons. For example, the $(2p3p)^3P$ state is bound because $(1s\varepsilon\ell)$ cannot couple to a ${}^3P^e$ state. Other states are very narrow, e.g., the first ${}^3D^e$ state in Table IV has a width of only 3×10^{-8} a.u. These states can be studied with optical methods since the radiative decay is a competitive or the dominant process. In Table VIII the calculated results are compared with some measured transition wavelengths [57] and widths [58]. The transition wavelengths agree very well.

For the widths the experimental situation is more complicated. Since for the 2364 Å $[(2s2p)^3P$–$(2p3p)^3P]$ as well as for the 2578 Å $[(2s2p)^3P$–$(2\ell3\ell')^3D^e]$ transition the upper state is of zero, $(2p3p)^3P$, or negligible, $(2\ell3\ell')^3D^e$, width, it is expected that the width for the transitions should be completely dominated by the width of the lower state $(2s2p)^3P$. In energy units the widths of 3.20 Å and 4.46 Å correspond to 7.10 ± 0.12 meV and 8.32 ± 0.08 meV, respectively; thus the two measurements of the width of the $(2s2p)^3P$ state give two different answers.

In Ref. [58] also the transition $[(2s2p)^3P$–$(2\ell4\ell')^3D^e]$, 2082 Å, is measured. Again the transition width should be given by the width of the $(2s2p)^3P$ state. Here the result is 2.90 ± 0.06 Å or 8.29 ± 0.15 meV, which thus supports the result from the $[(2s2p)^3P$–$(2\ell3\ell')^3D^e]$ transition

The width obtained here is 8.14 meV (corresponding to transition widths of 3.67 Å, 4.36 Å, and 2.84 Å) and very similar results are obtained by other calculations as can be seen in Table I. This gives further support to the conclusion that the width of the $(2s2p)^3P$ state is around 8 meV. There is at present no explanation for the appar-

TABLE VIII. Comparison between the present results and some beam-foil experiments, which measure the transition wavelengths between doubly excited states in He. The results are given in Å.

	Present[a]		Experiment			
	E	Γ	E		Γ	
$(2s2p)^3P$–$(2p3p)^3P$	2364.3[a]	3.67	2364.0	±0.5[b]		
					3.20	±0.05[c]
$(2s2p)^3P$–$(2\ell3\ell')^3D^e$ (1)	2578.0[a]	4.36	2577.6	±0.5[b]		
					4.46	±0.04[c]
$(2p2p)^3P$–$(2\ell3\ell')^3P^o$ (3)	2818.0[a]	0.00028	2817.6	±0.5[b]		
$(2p2p)^3P$–$(2\ell3\ell')^3D^o$ (2)	3013.5[a]		3013.0	±1.0[b]		

[a] The results from Tables I and IV. To convert the energy differences to transition wavelengths, λ, we use λ (Å) $= 455.5505/\Delta E$ (a.u.). The number in parentheses tells if it is the first, second, or third state of a particular symmetry which is used.

[b] Brooks and Pinnington [57].

[c] Cedequist *et al.* [58].

ently too narrow experimental width of the $(2s2p)^3P$–$(2p3p)^3P$ transition [59].

V. CONCLUSIONS

It has been shown that it is possible to describe doubly excited states accurately with finite discrete basis sets combined with complex rotation. The results presented here agree well with the most accurate earlier calculations available, which uses Hylleraas wave functions.

The method described here can easily be applied to larger systems than helium along the same lines as the bound-state scheme was extended from helium to other systems. The use of, e.g., a Hartree-Fock basis set requires though an iterative scheme to obtain the rotated Hartree-Fock potential. The extension to relativistic systems cause no special problems either. The complex rotation of the one-particle Dirac equation is as straightforward as the complex rotation of the one-particle Schrödinger equation.

ACKNOWLEDGMENTS

I am grateful for valuable discussions with Dr. A.-M. Mårtensson-Pendrill, Dr. S. Salomonson, Dr. N. Elander, and Professor G. Drake. Financial support was received from the Swedish Natural Science Research Council (NFR).

---

[1] A. K. Bhatia and A. Temkin, Phys. Rev. A **11**, 2018 (1975).
[2] A. K. Bhatia and A. Temkin, Phys. Rev. A **29**, 1895 (1984).
[3] D. H. Oza, Phys. Rev. A **33**, 824 (1986).
[4] Y. K. Ho, J. Phys. B **12**, 387 (1979).
[5] Y. K. Ho, Phys. Rev. A **23**, 2137 (1981).
[6] Y. K. Ho, J. Phys. B **15**, L691 (1982).
[7] Y. K. Ho and J. Callaway, Phys. Rev. A **27**, 1882 (1983).
[8] Y. K. Ho and J. Callaway, J. Phys. B **18**, 3481 (1985).
[9] Y. K. Ho, Phys. Rev. A **34**, 4402 (1986).
[10] Y. K. Ho, Z. Phys. D **21**, 191 (1991).
[11] Y. K. Ho and A. K. Bhatia, Phys. Rev. A **44**, 2895 (1991).
[12] Y. K. Ho, Phys. Rev. A **44**, 4154 (1991).
[13] Y. K. Ho, Phys. Rev. A **48**, 3598 (1993).
[14] Y. K. Ho and A. Bhatia, Phys. Rev. A **47**, 2628 (1993).
[15] K. T. Chung and B. F. Davis, Phys. Rev. A **26**, 3278 (1982).
[16] C. Froese-Fischer and M. Idrees, J. Phys. B **23**, 679 (1990).
[17] J. Tang, S. Watanabe, and M. Matsuzawa, Phys. Rev. A **46**, 2437 (1992).
[18] D. R. Herrick and O. Sinanoglu, Phys. Rev. A **11**, 97 (1975).
[19] U. Fano, Rep. Prog. Phys. **46**, 97 (1983).
[20] C. D. Lin, Phys. Rev. A **29**, 1019 (1984).
[21] A. R. P. Rau, J. Phys. B **16**, L699 (1983).
[22] S. Salomonson and P. Öster, Phys. Rev. A **40**, 5559 (1989).
[23] S. Salomonson and P. Öster, Phys. Rev. A **40**, 5548 (1989).
[24] W. R. Johnson, S. A. Blundell, and J. Sapirstein, Phys. Rev. A **37**, 307 (1988).
[25] S. Salomonson and P. Öster, Phys. Rev. A **41**, 4670 (1990).
[26] A.-M. Mårtensson-Pendrill and A. Ynnerman, Phys. Scr. **41**, 329 (1990).
[27] S. Salomonson and A. Ynnerman, Phys. Rev. A **43**, 88 (1991).
[28] A.-M. Mårtensson-Pendrill *et al.*, J. Phys. B **23**, 1749 (1990).
[29] E. Lindroth and S. Salomonson, Phys. Rev. A **41**, 4659 (1990).
[30] E. Lindroth, H. Persson, S. Salomonson, and A.-M. Mårtensson-Pendrill, Phys. Rev. A **45**, 1493 (1991).
[31] E. Lindroth and J. Hvarfner, Phys. Rev. A **45**, 2771 (1991).
[32] E. Lindroth and A. Ynnerman, Phys. Rev. A **47**, 961 (1993).
[33] A.-M. Mårtensson-Pendrill, D. S. Gough, and P. Hannaford, Phys. Rev. A **49**, 3351 (1994).
[34] R. M. Lowe, P. Hannaford, and A.-M. Mårtensson-Pendrill, Z. Phys. D **28**, 283 (1993).
[35] G. W. F. Drake, Nucl. Instrum. Methods Phys. Res. B **31**, 7 (1988).
[36] For an account of the early contributions to the complex rotation method see the whole issue of Int. J. Quantum Chem. **14** (4) (1978).
[37] T. N. Rescigno and V. McKoy, Phys. Rev. A **12**, 522 (1975).
[38] Y. K. Ho, J. Phys. B **10**, L373 (1977).
[39] I. Lindgren, J. Phys. B **7**, 2441 (1974).
[40] S. Salomonson, I. Lindgren, and A.-M. Mårtensson, Phys. Scr. **21**, 351 (1980).
[41] C. D. Lin and J. H. Macek, Phys. Rev. A **29**, 1019 (1984).
[42] A. K. Bhatia, Phys. Rev. A **2**, 1667 (1970).
[43] K. E. Banyard, D. R. T. Keeble, and G. W. F. Drake, J. Phys. B **25**, 3405 (1992).
[44] D. R. T. Keeble, K. E. Banyard, and G. W. F. Drake, J. Phys. B **26**, 2811 (1993).
[45] R. P. Madden and K. Codling, Phys. Rev. Lett. **10**, 516 (1963).
[46] R. P. Madden and K. Codling, Astrophys. J. **141**, 364 (1965).
[47] P. Dhez and D. L. Ederer, J. Phys. B **6**, L59 (1973).
[48] H. D. Morgan and D. L. Ederer, Phys. Rev. A **29**, 1901 (1984).
[49] H. Kossmann, B. Krässig, and V. Schmidt, J. Phys. B **21**, 1489 (1988).
[50] M. Zubek, G. C. King, P. Rutter, and F. Read, J. Phys. B **22**, 3411 (1989).
[51] M. Domke *et al.*, Phys. Rev. Lett. **66**, 1306 (1991).
[52] G. W. F. Drake, Can. J. Phys. **66**, 586 (1988).
[53] W. R. Johnson and G. Soff, At. Data Nucl. Data Tables **33**, 405 (1985).
[54] K. T. Chung and B. F. Davis, Phys. Rev. A **31**, 1187 (1985).
[55] P. J. Hicks and J. Comer, J. Phys. B **8**, 1866 (1975).
[56] F. Gelebart, R. J. Tweed, and J. Peresse, J. Phys. B **9**, 1739 (1976).
[57] R. L. Brooks and E. H. Pinnington, Phys. Rev. A **22**, 529 (1980).
[58] H. Cederquist, M. Kisielinski, and S. Mannervik, J. Phys. B **16**, L479 (1983).
[59] S. Mannervik (private communication).