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Saddle-point technique for helium in the elastic- and inelastic-scattering energy region

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The saddle-point technique is applied to the helium atom below the ionization threshold and for ^1P and ^3P resonances in the elastic-, and inelastic-scattering energy region. The results generally support the assertion that the method gives the best square-integrable approximation within the inner-shell vacancy picture for excited or autoionizing states. For the resonance where the Feshbach shift is negative, the saddle-point method gives essentially the same result as that of the QHQ approximation. However, for resonances with a large positive Feshbach shift, the results of the new method are substantially better. For example, for the lowest ^1P resonance in the inelastic-scattering region, we get 69.901 eV, the experimental result is 69.90 ± 0.04 eV by Madden and Codling, 69.92 ± 0.03 eV by Dhez and Ederer.

I. INTRODUCTION

The inner-shell vacancy states of a quantum system have generated great interest in the past. Experimentally, they correspond to the discrete spectrum of the system embedded in the continuum.[1] They exist in atomic, molecular, nuclear, and solid systems. These states arise in collision, photoabsorption, nuclear decay, as well as elementary-particle capture. Once formed, they may decay through many different channels such as autoionization, x-ray emission, Coster-Kronig transition, etc.[2] Many theoretical methods have been developed to study these states, especially for atomic systems with a few particles. For example, the close-coupling method,[3] the Feshbach projection-operator method,[4] the complex-rotation method,[5] and the quasi-projection-operator method,[6] etc. However, each method has its own limitations in dealing with the highly excited states of a complicated system.

Recently, a new variational method[7] has been developed to calculate the energy and wave function of an inner-shell vacancy system. This method is comparitively simple to use. There are no restrictions as to the number of particles or the number of vacancies within the system.

The basic assumption in this method is that a vacancy in a many-electron system can be represented by a single-particle orbital $\phi_0(\vec{r})$. In a variational calculation, one uses a multiconfiguration trial wave function

$$\Psi = A\psi(\vec{r}_1, \vec{r}_2, \ldots, \vec{r}_j, \ldots \vec{r}_n)\,, \tag{1}$$

where A is an antisymmetrization operator. If electron j in the wave function ψ has the same symmetry as ϕ_0 and it is the only particle that may fill the vacancy, then an n-electron wave function containing a ϕ_0 vacancy is

$$\Psi' = A[1 - P_0(\vec{r}_j)]\psi(\vec{r}_1, \vec{r}_2, \ldots, \vec{r}_j, \ldots \vec{r}_n)\,, \tag{2a}$$

where

$$P_0(\vec{r}) = |\phi_0(\vec{r})\rangle\langle\phi_0(\vec{r})|\,. \tag{2b}$$

If Eqs. (2) are used with the Rayleigh-Ritz variation method, the lowest eigenvalue will correspond to the lowest state with that vacancy. The higher eigenvalues approximate the higher excited states in accordance with MacDonald's theorem.[8]

The question is therefore how to make an intelligent choice of $\phi_0(\vec{r})$. In Ref. 7, a theorem is proved which shows that if one parametrizes ϕ_0, then the energy of the inner-shell vacancy state corresponds to the saddle-point solution in the Rayleigh-Ritz variation method. That is, it is a minimum with respect to the parameters in ψ and a maximum with respect to the parameters in ϕ_0. It is also shown in this reference that the solution so obtained should be the best possible square-integrable solution to the problem of interest.

In this work, we test this theorem by using the $e + \mathrm{He}^+$ system for three energy regions: below the ionization threshold, in the elastic-scattering region, and in the inelastic region. The reason that this particular system is chosen is partly because other accurate theoretical and experimental data are available for comparison, thus providing an unambiguous test of the saddle-point technique. In Sec. II, the trial wave function is given along with a description of the procedure used. Section III specializes to single-particle excitation. Since these energies can be accurately calculated with MacDonald's theorem, the two results will be compared. Section IV deals with the ^1P and ^3P doubly excited states of He in the $n=1$ to $n=2$ energy region. These results are compared with the accurate Feshbach calculation[9] and with experiment.[10] Section V gives the ^1P and ^3P excited states in the $n=2$ to $n=3$ energy region. Previously, disagreement existed between the experimental result[10,11] and the Feshbach QHQ calculation.[12] However, by using the saddle-point technique the new theoretical result gives excellent agreement with the experiment. Section VI is a brief summary.

II. WAVE FUNCTION AND PROCEDURE

In atomic units the nonrelativistic Hamiltonian for a two-electron atomic system is

$$H=-\tfrac{1}{2}\nabla_1^2-\tfrac{1}{2}\nabla_2^2-Z/r_1-Z/r_2+1/r_{12}\,. \tag{3}$$

To solve for the energy states of this Hamiltonian, we use a variation method. A set of basis functions is chosen for the expansion. The spacial part of the basis function is given by the product of

$$\phi_{ij}(r_1,r_2)=r_1^i r_2^j e^{-(\alpha r_1+\beta r_2)}\,, \tag{4a}$$

$$|LMl_1l_2\rangle=\sum_{m_1m_2}\langle l_1l_2m_1m_2|LM\rangle Y_{l_1m_1}(\hat{r}_1)Y_{l_2m_2}(\hat{r}_2)\,. \tag{4b}$$

For the system of interest, the LS coupling scheme is used. Therefore the total wave function is given by the simple product of the spacial part and the spin part $\chi(1,2)$, which takes the form of either a singlet or triplet.[13] Thus the trial wave function is given by

$$\begin{aligned}\Psi&=A\sum_{ij,l_1l_2}C_{ijl_1l_2}\phi_{ij}(r_1,r_2)|LMl_1l_2\rangle\chi(1,2)\\&=A\psi(\vec{r}_1,\vec{r}_2)\,.\end{aligned} \tag{5}$$

To build vacancies into the total wave function, we choose

$$\phi_{nlm}(\mathbf{r})=NR_{nl}(r)Y_{lm}(\theta,\phi)\,, \tag{6a}$$

where

$$R_{nl}^{(r)}=e^{-qr/n}\left(\frac{2qr}{n}\right)^l L_{n+l}^{2l+1}\left(\frac{2qr}{n}\right), \tag{6b}$$

and N is a normalization constant, L_{n+l}^{2l+1} is the associated Laguerre polynomial, and q is a nonlinear parameter to be determined by optimization. This form of ϕ_0 is chosen partly because of its simplicity and partly because of its physical plausibility.

If the two-electron system is in the elastic-scattering energy region, a wave function containing a $1s$ vacancy is given by

$$\Psi=A[1-P_{1s}(\vec{r}_1)][1-P_{1s}(\vec{r}_2)]\psi(\vec{r}_1,\vec{r}_2)\,, \tag{7a}$$

where

$$P_{1s}(\vec{r})=|\phi_{1s}(\vec{r})\rangle\langle\phi_{1s}(\vec{r})|\,. \tag{7b}$$

In carrying out the Rayleigh-Ritz variation procedure, the energy E is minimized first with respect to C to obtain the secular equation. The eigenvalues are then minimized with respect to α and β, and maximized with respect to q.

It is well known that the Feshbach formalism[4] provides an exact formulation for two-electron scattering systems. In this formulation the Hilbert space is divided into open and closed channels with the corresponding projection operators P and Q. Hence the Schrödinger equation becomes

$$\left(PHP-PHQ\frac{1}{QHQ-E}QHP-E\right)P\Psi=0\,. \tag{8}$$

It is clear from this equation that resonances arise when E approaches an eigenvalue of the QHQ operator. It can be shown that if

$$(QHQ-\epsilon_n)\phi_n=0\,, \tag{9}$$

then the Feshbach resonance energy associated with this ϵ_n is given by[14]

$$E_{\text{res}}=\epsilon_n+\Delta_n(E_{\text{res}})\,, \tag{10}$$

where Δ_n is a shift due to the coupling of ϕ_n and the rest of the Hilbert space through the total Hamiltonian. It is shown by Hahn *et al.*[15] that the Q operator for the two-electron system in the elastic scattering region is given by

$$Q\Psi=[1-P_{1s}(\vec{r}_1)][1-P_{1s}(\vec{r}_2)]\Psi\,. \tag{11}$$

This Q operator is identical to that of Eq. (7a) except that it is strictly hydrogenic and contains no parameters. This provides a particularly interesting test of the present method. The saddle-point technique maximizes the energy with respect to the parameters in the vacancy orbitals, so in general the saddle-point energy will be higher than ϵ_n. If Δ_n in Eq. (10) is positive, the saddle-point solution will probably provide a better result than ϵ_n. However, it is known that in some rare cases Δ_n is negative,[9] so it appears that in these instances the QHQ approximation, ϵ_n, may give a better result. This will be studied in detail in Sec. IV.

III. SINGLY EXCITED BOUND STATES

From a mathematical point of view, the time-independent Schrödinger equation is an eigenvalue equation with discrete as well as continuous eigenvalues and eigenfunctions. On the other hand, one visualizes the physical system as consisting of individual particles each occupying a certain orbit. One describes the system in terms of particle excitation and interprets the energy states in terms of various configurations. It would be interesting to know how accurate this description actually is. The saddle-point technique provides a means to make such an analysis. For example, the 2nd-lowest eigenvalue of helium with singlet spin is interpreted to be the $(1s2s)\,^1S$ state. Using the saddle-point technique we can build a $1s$ vacancy in the He wave function and solve for the lowest singlet energy state with this vacancy. The accuracy of the new result gives a measure of the adequacy of the $1s2s$ interpretation. To make this comparison, the eigenvalue of the Hamiltonian is computed by searching for the minimum value of the 2nd-lowest root in the Rayleigh-Ritz variation method using an unprojected wavefunction.

For the $(1s2s)\,^1S$ state, $L=0$ and $M=0$. Following Eq. (4), the basis function can be written as

$$\phi_{lij}(\vec{r}_1, \vec{r}_2) = \phi(r_1, r_2)\,|00ll\rangle\,. \tag{12}$$

The trial function takes the form

$$\Psi = A \sum_{lij} C_{lij}\phi_{lij}(\vec{r}_1, \vec{r}_2)\,. \tag{13}$$

We begin by taking a $l=0$, 15 term trial function. α is fixed at the hydrogenic value of 2.0 and β is varied. The best energy is $-2.144\,113$ a.u. at $\beta=0.80$. This energy will be denoted by $\epsilon^{(1)}$ where the superscript gives the number of angular partial waves l included. If an $l=1$, 10 term basis is added, $\epsilon^{(2)}$ becomes $-2.145\,353$ a.u. at $\beta=0.86$. With another 6 term $l=2$ basis, $\epsilon^{(3)}=-2.145\,391$ a.u. at $\beta=0.86$. The "exact" value of Perkeris[16] for this state is $-2.145\,974$ a.u.

To search for the saddle-point energy, we assume for the normalized vacancy orbital

$$\phi_0(r) = (1/\sqrt{\pi})q^{3/2}e^{-qr}\,, \tag{14}$$

where q is a parameter to be optimized. The trial function takes the form

$$\Psi' = A \sum_{lij} C_{lij}[1 - P_0(\vec{r}_2)]\phi_{lij}(\vec{r}_1, \vec{r}_2)\,. \tag{15}$$

By using the same number of terms in the trial functions as before we calculate the lowest eigenvalue $\lambda^{(1)}$, we find $\lambda^{(1)}=-2.144\,095$ a.u. at $\beta=0.86$, $\lambda^{(2)}=2.145\,366$ a.u., and $\lambda^{(3)}=-2.145\,406$ a.u. at $\beta=0.90$. All three saddle points occur at $q=1.52$. Define the corresponding Rayleigh-Ritz energy with the same β as the saddle point to be $E^{(1)}$, $E^{(2)}$, and $E^{(3)}$, we find $E^{(1)}=-2.144\,089$ a.u., $E^{(2)}=-2.145\,334$ a.u., and $E^{(3)}=-2.145\,373$ a.u. The differences between λ and E, or λ and ϵ, all occur at the sixth or seventh digit. A similar calculation is also done for Li^+ and Be^{++} systems.

To see whether the same accuracy can be achieved for other angular orbitals, the $He(1s3p)\,^3P$ state is investigated by building a $2p$ vacancy in the $(1snp)\,^3P$ wave function in the calculation. These results are given in Table I. For all systems considered in this table, the disagreements all appear at the sixth or seventh digit. In all cases the saddle point is very easy to find. In Table II, the energy around the saddle point of $Li^+(1s2s)\,^1S$ is given. In this table, the highest energy for each β and different q is underlined, the lowest energy for each q and different β is indicated by a check mark. The saddle point is where they meet.

It would be of interest to see whether the saddle points for the higher states of this system occur at the same q. The calculation for $He(1s3s)\,^1S$ again gives $q=1.52$, suggesting that

$$\phi_0 = (1/\sqrt{\pi})(1.52)^{3/2}e^{-1.52r}$$

is probably a good approximation to the vacant $1s$ orbital for this system. In this calculation a 21 term $l=0$ and 15 term $l=1$ trial function is used. Here $\lambda^{(1)}=-2.060\,712$ a.u., $\lambda^{(2)}=-2.060\,794$ a.u.,

TABLE I. Comparison of the saddle-point energy and the energy of an unprojected wave function (in a.u.). For notation in the first column, see text. For $He(1s3p)\,^1P$, the trial function includes up to two angular partial waves, a 19 term s-p wave and a 10 term p-d wave.

State	$He(1s2s)\,^1S$	$He(1s3p)\,^3P$	$Li^+(1s2s)\,^1S$	$Be^{++}(1s2s)\,^1S$
λ^1	$-2.144\,095$	$-2.057\,731$	$-5.037\,560$	$-9.180\,608$
ϵ^1	$-2.144\,113$	$-2.057\,747$	$-5.037\,559$	$-9.180\,601$
E^1	$-2.144\,089$	$-2.057\,747$	$-5.037\,553$	$-9.180\,601$
$\lambda^1-\epsilon^1$	1.8×10^{-5}	1.6×10^{-5}	-0.1×10^{-5}	-0.7×10^{-5}
λ^1-E^1	-0.6×10^{-5}	1.6×10^{-5}	-0.7×10^{-5}	-0.7×10^{-5}
λ^2	$-2.145\,366$	$-2.057\,894$	$-5.039\,907$	$-9.183\,645$
ϵ^2	$-2.145\,353$	$-2.057\,911$	$-5.039\,889$	$-9.183\,630$
E^2	$-2.145\,334$	$-2.057\,911$	$-5.039\,884$	$-9.183\,624$
$\lambda^2-\epsilon^2$	-1.3×10^{-5}	1.7×10^{-5}	-1.8×10^{-5}	-1.5×10^{-5}
λ^2-E^2	-3.2×10^{-5}	1.7×10^{-5}	-2.3×10^{-5}	-2.1×10^{-5}
λ^3	$-2.145\,406$		$-5.040\,020$	$-9.183\,821$
ϵ^3	$-2.145\,391$		$-5.040\,000$	$-9.183\,804$
E^3	$-2.145\,373$		$-5.039\,997$	$-9.183\,800$
$\lambda^3-\epsilon^3$	-1.5×10^{-5}		-2.0×10^{-5}	-1.7×10^{-5}
λ^3-E^3	-3.3×10^{-5}		-2.3×10^{-5}	-2.1×10^{-5}

TABLE II. Saddle-point energy technique for $2\,^1S_0$ of Li^+ (in a.u.). The numbers given here are the last three digits from a seven significant figure energy. The first four digits are identical. The underline gives the highest value for each nonlinear parameter β, the check mark gives the lowest energy for each q. The saddle point is where they meet. N is the number of terms in the trial function. For notations see text. α is fixed at 3.00.

β						E			
q	1.47	1.50	1.53	1.56	1.59	1.62	1.65	N	Saddle-point energy
2.505	709	717	720 ✓	717	705				
2.520	598	604	608 ✓	604	591				
2.535	$\underline{551}$	$\underline{558}$	$\underline{560}$ ✓	$\underline{555}$	$\underline{542}$			15	−5.037 560
2.550	566	573	574 ✓	569	555				
2.565	641	647	648 ✓	642	628				
2.532			908	923	930 ✓	927	911		
2.538			892	907	913 ✓	910	894		
2.544			$\underline{886}$	$\underline{901}$	$\underline{907}$ ✓	$\underline{903}$	$\underline{886}$	25	−5.039 907
2.550			890	905	910 ✓	906	889		
2.556			904	918	924 ✓	919	901		
2.532			017	034	043 ✓	041	027		
2.538			002	018	026 ✓	024	010		
2.544			$\underline{000}$	$\underline{012}$	$\underline{020}$ ✓	$\underline{017}$	$\underline{002}$	31	−5.040 020
2.550			000	016	023 ✓	020	005		
2.556			015	030	037 ✓	033	018		

$E^{(1)}=-2.060\,741$ a.u., and $E^{(2)}=-2.060\,824$ a.u. Again differences occur at the sixth digit.

It is interesting to note that for the helium system a $q=1.52$ implies the vacancy feels the presence of the other 1s electron. The vacancy orbital is approximately half screened by this electron.

IV. ^1P AND ^3P RESONANCES IN THE He^+ $n=1$ to $n=2$ ENERGY REGION

To test the effectiveness of the saddle-point technique, the ^1P resonances of He are particularly well suited for three reasons. First of all, the Feshbach projection-operator calculation has been carried out accurately for this system, providing a meaningful comparison to the new method. Second, accurate experimental results are available for the higher members of the resonances. Third, the Feshbach shift of the lowest ^1P resonance is known to be negative even for an Hylleraas-coordinate wave function.[17] Since the saddle-point solution is always higher than or at least equal to the eigenvalue of QHQ, it would be interesting to find out if the solution for this resonance is inferior to that of QHQ. If true, it would contradict the assertion that the saddle-point solution provides the best square-integrable wave function approximation to the autoionizing state.

The configurations of ^1P resonances has been analyzed by Cooper and Fano,[18] the two principal series are classified as the plus and minus series with the configuration of $2snp \pm 2pns$. This is used to explain the experimental observations of Madden and Codling.[10] The third series which is mainly a mixture of the $2snp+2pnd$ configuration, called the pd series, has also been found to contribute to the observed spectrum.[19] To calculate the energies with the saddle-point method, we use Eqs. (4) and (5) for the trial function, Eq. (14) for the 1s vacancy, and Eq. (7) for the projected trial function. We fix $\alpha=1$ which is the proper hydrogenic value and search for a minimum of energy for β and a maximum for q. For the lowest ^1P resonance, 76 linear parameters and five angular partial waves are used. For higher resonances, either 78 terms with three partial waves or 77 terms with two partial waves are used, depending on which choice gives a better energy. These results are given in Table III.

In this table, the lowest eight ^1P resonances from the saddle-point solution and the eigenvalues ϵ_n of QHQ are compared. For the lowest resonance, the difference between the two solutions occurs at the seventh digit. This seems to suggest that when the Feshbach shift is negative, the saddle-point solution will be essentially identical to that of the QHQ solution. The Feshbach shift of the second and third resonances is calculated by Bhatia and Temkin to be positive and negative, respectively; this also agrees with the saddle-point solutions. For higher resonances, our calculations show the saddle point occurring at $q=2.00$, hence the saddle-point solution is identical to the QHQ approximation. Except for the 2nd resonance, the two methods give the same result. The Feshbach shifts of some of the higher reso-

TABLE III. ^1P resonances of $e+\mathrm{He}^+$ in the $n=1$ to $n=2$ energy region (in a.u.). ϵ_n is the QHQ energy. E_n is the saddle-point energy. Δ is the Feshbach shift from Ref. 9. $E_{\max}$ (from Ref. 10) differs from the resonance position by width/(2 × line profile). The figure in the parentheses gives the uncertainty quoted. The conversion factor used is $E=455.696/\lambda$ where λ is in Å. For β and q, see Eqs. (4) and (6). $\alpha=1.00$.

Series	β	$-\epsilon_n$	$-E_n$	q	$E_n-\epsilon_n$	Δ	$-E_{\max}$(expt.)
+	1.15	0.692 660 3	0.692 659 5	1.99	8×10^{-7}	-2.6×10^{-4}	0.693 86 (54)
−	0.62	0.597 091	0.597 078	1.98	1.3×10^{-5}	2.3×10^{-5}	0.597 10 (35)
+	0.54	0.563 861	0.563 861	2.00	0	-7.4×10^{-5}	0.564 18 (24)
−	0.41	0.547 017	0.547 017	2.00	0		0.546 27 (61)
pd	0.40	0.546 411	0.546 411	2.00	0		
+	0.37	0.534 129	0.534 129	2.00	0		0.534 38 (25)
−	0.28	0.527 492	0.527 492	2.00	0		0.526 97 (62)
pd	0.27	0.527 222	0.527 222	2.00	0		

nances are calculated by Burke and McVicar[20] and are shown to be very small. It is well known that this shift depends a great deal on the wave function used, so unless the unshifted energies of the two calculations have comparable accuracy, an absolute comparison of the shifts is meaningless.

Contrary to the ^1P calculation, the ^3P resonance calculation shows substantial differences between the saddle-point solution and the QHQ approximation. This is especially true for the lower resonances (see Table IV). The differences are less than the full shifts calculated by Bhatia and Temkin. This seems to suggest that the saddle-point method does not "over correct" the QHQ approximation. Four ^3P resonances are observed by Rudd,[21] the results of this work lie well within the experimental error quoted for these four states.

One interesting feature in this table is that for each resonant series, q approaches the hydrogenic value 2.00 monotonically as the resonance energy gets higher. The different ways in which q approaches its limit indicates that the intrinsic structure, or the shielding of the nucleus might be different for each series.

V. ^1P AND ^3P RESONANCES IN THE He^+ $n=2$ to $n=3$ ENERGY REGION

In this energy region, the $1s$, $2s$, $2p$ channels of He^+ become open. The trial wave function for the Feshbach resonances takes the form

$$\Psi'=A[1-|P(1)\rangle\langle P(1)|][1-|P(2)\rangle\langle P(2)|]\psi(\vec{r}_1,\vec{r}_2)\,, \tag{16a}$$

where

$$P(i)=\sum_{n=1}^{2}\sum_{l=0}^{n-1}\sum_{m=-l}^{l}|\phi_{nlm}(\vec{r})\rangle\langle\phi_{nlm}(\vec{r})|\,, \tag{16b}$$

and ϕ_{nlm} is given by Eq. (6).

Theoretically the ^1P resonances in this energy region have been calculated by Oberoi[22] and by Chung[12] using the QHQ approximation of Feshbach, by Burke and Taylor[23] using a close-coupling calculation with three-state plus correlation, by Herrick and Sinanoglu[24] using a group-theoretical method, and more recently by Ho[25] using a complex-rotation method. Experimental results have been given by Madden and Codling[10] and by Dhez

TABLE IV. ^3P resonances of $e+\mathrm{He}^+$ in the $n=1$ to $n=2$ energy region (in a.u.). For notation see Table III. 1 a.u. = 27.211 65 eV is used in the conversion (see Ref. 9). $\alpha=1.00$.

Series	β	$-\epsilon_n$	$-E_n$	q	$E_n-\epsilon_n$	Δ [a]	$-E$(expt.) [b]
−	1.15	0.761 457	0.760 842	1.92	0.62×10^{-3}	1×10^{-3}	0.7598 (18)
−	0.61	0.584 888	0.584 822	1.97	0.66×10^{-4}	2.7×10^{-4}	0.5856 (18)
+	0.58	0.579 006	0.579 006	2.00	0	2.7×10^{-6}	
pd	0.47	0.548 763	0.548 758	2.01	5×10^{-6}		
−	0.42	0.542 851	0.542 842	1.99	9×10^{-6}		0.5437 (18)
+	0.37	0.539 494	0.539 494	2.00	0		
pd	0.33	0.528 489	0.528 488	2.01	10^{-6}		
−	0.28	0.525 666	0.525 665	1.99	10^{-6}		0.5257 (18)
+	0.27	0.523 862	0.523 862	2.00	0		

[a] Reference 9.

[b] Reference 21.

TABLE V. ^1P resonances of $e+\mathrm{He}^+$ in the $n=2$ to $n=3$ energy region (in a.u.). ϵ_n is the QHQ energy, E_n is the saddle-point energy. $E_{\max}$ (from Ref. 10) is the position of maximum absorption-line intensity which differs from the resonance position by width/(2 × line profile). In the case of the lowest resonance this shifts the resonance position to −0.334 68 (145) a.u. (see Ref. 11). The figure in the parentheses gives the uncertainty in the last three digits quoted. $\alpha=\frac{2}{3}$ is used.

Series	β	$-\epsilon_n$	$-E_n$	q	$E_n-\epsilon_n$	$-E_{\max}$(Expt.)
+	0.71	0.335 827	0.334 597	1.87	1.23×10^{-3}	0.332 95 (145)
A	0.39	0.286 020	0.285 971	1.97	4.9×10^{-5}	
B	0.46	0.282 840	0.282 789	2.04	5.1×10^{-5}	
+	0.36	0.271 126	0.270 891	1.92	2.35×10^{-4}	0.269 80 (46)
C	0.38	0.267 505	0.267 499	1.99	6×10^{-6}	
A	0.26	0.257 441	0.257 430	1.98	1.1×10^{-5}	
B	0.26	0.251 206	0.251 204	2.01	2×10^{-6}	
+	0.24	0.250 481	0.250 433	1.96	4.8×10^{-5}	0.249 85 (46)
C	0.22	0.248 004	0.248 004	2.00	0	
D	0.21	0.244 915	0.244 893	2.03	2.2×10^{-5}	

and Ederer.[11]

By utilizing Eqs. (4), (6), and (16) in a Rayleigh-Ritz variation method, the saddle-point energy is sought. For the lowest ^1P resonance, 76 linear parameters and five angular partial waves are used. For higher members of the resonance series a three partial wave, 75 linear parameter wave function is used. The results are given in Table. V.

In this table, we see that unlike the ^1P states in the elastic-scattering region, the saddle-point solution gives a substantial improvement over the Feshbach QHQ energy. For example, the lowest resonance was somewhat below the experimental results. But the saddle-point solution, −0.334 597 a.u., is 69.901 eV above the ground state of helium and agrees excellently with the 69.92 ± 0.03 eV result of Dhez and Ederer[11] and the 69.90 ± 0.04 eV result of Madden and Codling.[10] The latter result, quoted from Ref. 11, is different from that of Table V, in which the position of maximum absorption-line intensity is given. Note that $E_{\mathrm{res}} = E_{\max} - \Gamma/2g$,[18] where Γ is the width of the resonance, and g is its line-profile parameter. Since Γ and g are not available for the higher resonances, we only quote $E_{\max}$ in this table. However, since the widths of the higher resonances are substantially narrower, $E_{\max}$ should be a better approximation to E_{res}.

There are five ^1P resonance series in this energy region which come from linear combinations of $3snp$, $3pns$, $3pnd$, $3dnp$, and $3dnf$. These series are classified into (+), A, B, C, and D in accordance with Ref. 12. The lowest ten resonance states are given in Table V. The higher members have not been calculated since the q values will be very close to 2.00, and therefore the results will be very close to those of Ref. 12. It is evident, from inspection of the table, that the value of q approaches the hydrogenic value of 2.00 monotonically from the lowest resonance of each series. The (+) series is the only series observed experimentally. The saddle-point solutions for the lowest three resonances of this series are substantially closer to the experimental results than those of the QHQ approximation.

Our calculated energies for the ^3P autoionization states in this energy region are given in Table VI. These results are compared with the QHQ approximation of Chung.[12] Once again, the calculations in this energy region show a greater improvement in the energy as compared to the ^3P calculations in the elastic-scattering region (see Table IV).

For the higher ^1P and ^3P resonances in this energy region there are few theoretical results available with shifts included. Therefore we only make comparison with the lowest member of each symmetry. These are given in Table VII. From this

TABLE VI. ^3P resonances of $e+\mathrm{He}^+$ in the $n=2$ to $n=3$ energy region (in a.u.). For notation, see Table V. $\alpha=\frac{2}{3}$. The principal series is denoted as the (−) series in the same sense as Table IV.

Series	β	$-\epsilon_n$	$-E_n$	q	$E_n-\epsilon_n$
−	0.69	0.351 790	0.350 818	1.90	9.72×10^{-4}
A	0.62	0.310 951	0.310 721	1.93	2.30×10^{-4}
−	0.32	0.280 094	0.279 908	1.98	1.86×10^{-4}
B	0.34	0.278 847	0.278 802	1.96	4.5×10^{-5}
A	0.30	0.260 328	0.260 233	1.97	9.5×10^{-5}
C	0.26	0.258 022	0.257 908	2.03	1.14×10^{-4}
−	0.28	0.255 412	0.255 412	2.00	0
B	0.28	0.253 502	0.253 494	1.99	8×10^{-6}
D	0.23	0.245 307	0.245 292	2.02	1.5×10^{-5}

TABLE VII. The lowest ^1P and ^3P autoionizing state of He in the inelastic-scattering region (in eV). 1 a.u. = 27.207 95 eV, He ground state = −2.903 724 a.u. is used in the conversion.

State	Theory BT [a]	Ho [b]	Present work	Experiment MC [c]	DE [d]
^1P	69.917	69.873 ± 0.0014	69.901	69.90 ± 0.04	69.92 ± 0.03
^3P	69.482	69.471 ± 0.0028	69.459		

[a] Burke and Taylor, Ref. 23.

[b] Reference 25.

[c] Madden and Codling, Ref. 10.

[d] Dhez and Ederer, Ref. 11. References 12, 22, and 24 are not included in this table because the Feshbach shifts are not considered in these references.

table it is seen that for the ^1P resonance the agreement between accurate theoretical calculations and experiments is satisfactory. For the ^3P resonance, similar agreement is obtained between theoretical work, but no experimental result is available for comparison.

VI. SUMMARY AND DISCUSSION

In this work, we have demonstrated the effectiveness of the saddle-point technique by carrying out calculations for He in the bound state, elastic- and inelastic-scattering energy regions. The helium system was chosen partly because correlation effects are important in this system, and also since many theoretical and experimental results are available for comparison. In the bound-state calculation, it was shown that the method is capable of generating accurate results within the limits of the trial function used. In the elastic-scattering region, we find that when the Feshbach shift is large and positive, the saddle-point method improves the QHQ approximation by recovering a large part of the Feshbach shift. For example, for the lowest ^3P resonance, it recovers 62% of the shift. For negative Feshbach shifts, the new method gives results essentially identical to that of the QHQ approximation. In the case of the inelastic-scattering energy region, the improvement over the QHQ approximation becomes more substantial; this is apparent from both ^1P and ^3P calculations. It appears that the higher the energy region, the more effective the saddle-point technique becomes as compared with the QHQ approximation in comparing with experiment. Unlike the QHQ approximation, the utility of the saddle-point technique is more general, allowing calculations to be made for many-electron systems.

Compared with the complex-rotation method, the advantage of the present method is that maximizing and minimizing the eigenvalues of each resonance is easily carried out. A suitable, flexible trial function can be easily chosen. Hence not only the low-lying resonance can be calculated, but the higher resonances can also be calculated with even greater accuracy. The disadvantage of this method is that it does not yield the width of a resonance without introducing the continuum. It would be of great interest to combine the advantages of both methods. This will be the direction we will be pursuing in the near future.

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