Evaluation of high-level bound-bound and bound-continuum hydrogenic oscillator strengths by asymptotic expansion

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An asymptotic expansion due to Menzel and Pekeris [Mon. Not. R. Astron. Soc. **96**, 77 (1935); reprinted in *Selected Papers on Physical Processes in Ionized Plasma*, edited by D. H. Menzel (Dover, New York, 1962)] has been used to give a series expansion for the bound-bound and bound-continuum oscillator strengths. For the bound-bound transitions between the initial and final principal quantum numbers n and n', and for any n and n' considered, the oscillator strength is within 0.5% accuracy of the exact values. For the bound-continuum oscillator strength, and continuum energies $\varepsilon \leq 1$ Ry, the accuracy is better than 1%. For $n^2\varepsilon \gg 1$, the method of Menzel and Pekeris is inapplicable. Using an alternative method, an expansion in terms of n and ε is derived that gives the oscillator strength within 1% accuracy.

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I. INTRODUCTION

Radiative transition probabilities among high-lying Rydberg states are of interest in studying the atomic excited states produced by laser beams. In astrophysics, these probabilities are essential in the study of the radio recombination lines, and a knowledge of the recombination rates between electrons and ions, which contain as a factor the bound-continuum oscillator strength, is necessary for the study of the recombination spectra and ionization equilibrium between ions and neutrals in the ionosphere and gaseous nebulae.

Menzel took an early interest in evaluating the bound-bound, bound-continuum, and continuum-continuum hydrogenic oscillator strengths due to their astrophysical applications, and through a number of papers [1–3] extensively formulated and tabulated these quantities. References should also be given to Green, Rush, and Chandler [4], who tabulated the bound-bound oscillator strengths, and Karzas and Latter [5], who tabulated the bound-continuum oscillator strengths. Bessis, Bessis, and Hardinger [6] have found a closed expression in the form of multiple summations for the bound-bound oscillator strength. Similar work has been done by Hardinger, Bessis, and Bessis [7] for the bound-continuum oscillator strength. However, the last four works are limited to transitions among low-lying energy levels.

Menzel and Pekeris [1] applied the method of steepest descent to the evaluation of the bound-bound, bound-continuum, and continuum-continuum oscillator strengths for transitions between a lower level n and upper levels n' and ε, where n and n' are the initial and final principal quantum numbers, and ε is the energy of the electron in the continuum in Rydberg units. The solution is in the form of an expansion valid for $n \gg 1$, and $n/n' \ll 1$, or $n^2\varepsilon \ll 1$. An arithmetic error in their calculation has been corrected by Burgess [8]. With five terms in the expansion, agreement with the exact values is found to be within a few percent.

In this paper eight terms in the expansion are kept, and the resulting bound-bound oscillator strength for any n and n' considered is within 0.5% of the exact values, even for such low-lying transitions as $n=1$ to $n'=2$. For the bound-continuum transitions, and in the range $\varepsilon \leq 1$, the resulting oscillator strength for all possible transitions obtained here is less than 1% different from the exact values. For $\varepsilon \gg 1$, using a method independent of that of Menzel and Pekeris, values of the oscillator strengths for all transitions considered are within 1% of the exact values.

II. RESULTS AND DISCUSSION

The bound-bound oscillator strength $f(n,n')$ for a transition between the lower and upper principal quantum numbers n and n' of a hydrogenic atom is given by [9]

$$f(n,n')=\frac{2^5}{3n^2}\left|\frac{[(n-n')/(n+n')]^{2(n+n')}}{n^2n'^2(n^{-2}-n'^{-2})^3}\,\frac{\Delta(n,n')}{n'-n}\right| , \tag{1}$$

where

$$\Delta(n,n')=[F(-n,-n'+1,1,\chi)]^2-[F(-n',-n+1,1,\chi)]^2 ,$$
$$\chi=-\frac{4nn'}{(n-n')^2} , \tag{2}$$

where $F(\alpha,\beta,\gamma,\chi)$ is the hypergeometric function.

Using these expressions and the method of steepest descent, Menzel and Pekeris [1] derived an asymptotic series for the bound-bound, bound-continuum, and continuum-continuum oscillator strengths. When this series is evaluated up to eight terms, realizing that some terms drop out, for the bound-bound oscillator strength we find that

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TABLE I. A comparison of the five-term and eight-term approximations with the exact values of $f(n,n')$ [3,4], and $g_{\parallel}(n,\varepsilon)$ [5,10]. Numbers in brackets indicate powers of ten.

n	n'	ε (Ry)	Exact	5 terms	Error (%)	8 terms	Error (%)
1	2		4.162[−1]	3.980[−1]	−4.4[+0]	4.141[−1]	−5.0[−1]
2	3		6.408[−1]	6.277[−1]	−2.0[+0]	6.380[−1]	−4.4[−1]
5	6		1.231	1.215	−1.3[+0]	1.226	−4.1[−1]
5	40		1.500[−4]	1.499[−4]	−6.7[−2]	1.500[−4]	0.0
40	41		7.916	7.820	−1.2[+0]	7.879	−4.7[−1]
900	901		1.720[+2]	1.699[+2]	−1.2[+0]	1.712[+2]	−4.7[−1]
900	906		9.621[−1]	9.619[−1]	−2.1[−2]	9.621[−1]	0.0
1		0	7.973[−1]	7.776[−1]	−2.5[+0]	7.947[−1]	−3.3[−1]
1		10	9.264[−1]	1.083	1.7[+1]	9.369[−1]	1.1[+0]
5		0	9.358[−1]	9.351[−1]	−7.5[−2]	9.358[−1]	0.0
5		11.11	9.371[−1]	1.136	2.1[+1]	9.471[−1]	1.1[+0]
10		11.11	9.379[−1]	1.138	2.1[+1]	9.497[−1]	1.3[+0]
20		2.50	1.089	1.143	5.0[+0]	1.100	1.0[+0]
40		0.625	1.100	1.111	1.0[+0]	1.101	9.1[−2]
50		0.04	1.052	1.052	0.0	1.052	0.0

$$f(n,n')\cong\frac{2^6}{6\sqrt{3}\pi n^5 n'^3}\left[\frac{1}{n^2}-\frac{1}{n'^2}\right]^{-3}F(n,n')\ ,$$

$$\begin{aligned}F(n,n')=1&-0.172\,86\frac{AB^{-2/3}}{n^{2/3}}\\&-0.016\,531\,9\frac{B^{-4/3}C}{n^{4/3}}+\frac{1}{175}\frac{AB^{-2}C}{n^2}\\&+O(1/n^{8/3})\ ,\end{aligned}\qquad(3)$$

$$A=1+\alpha^2\ ,\quad B=1-\alpha^2\ ,\quad C=3-4\alpha^2+3\alpha^4\ ,$$

$$\alpha=n/n'\ll 1\ .$$

The first three terms in $F(n,n')$ are identical to those found by Menzel and Pekeris [1], taking into account the correction made by Burgess [8].

For the bound-continuum oscillator strength $f(n,\varepsilon)$, where ε is the energy of the continuum electron in Rydberg units, we let $n'\to i/\sqrt{\varepsilon}$. Taking the Coulomb normalization factor into account, we obtain for the bound-continuum Gaunt factor $g_{\parallel}(n,\varepsilon)$ the following expression:

$$g_{\parallel}(n,\varepsilon)\cong[1-\exp(-2\pi/\sqrt{\varepsilon})]^{-1}[F(n,n')]_{n'^2\to 1/\varepsilon}\ ,\qquad(4)$$

or

TABLE II. A comparison of the eight-term approximation of the asymptotic expansion (AEA) with the exact values of $f(n,n')$ [3,4]. Numbers in brackets indicate powers of ten.

		$f(n,n')$					$f(n,n')$		
n	n'	Exact	AEA	Error (%)	n	n'	Exact	AEA	Error (%)
1	2	4.162[−1]	4.141[−1]	0.50	10	11	2.190	2.180	0.46
	3	7.910[−2]	7.887[−2]	0.29		12	3.408[−1]	3.406[−1]	0.06
	10	1.605[−3]	1.600[−3]	0.31		20	5.468[−3]	5.468[−3]	0
	20	1.966[−4]	1.960[−4]	0.31		30	9.853[−4]	9.853[−4]	0
	30	5.809[−5]	5.787[−5]	0.38		40	3.556[−4]	3.556[−4]	0
	40	2.446[−5]	2.438[−5]	0.33	20	21	4.100	4.080	0.49
2	3	6.408[−1]	6.380[−1]	0.44		22	6.050[−1]	6.046[−1]	0.07
	4	1.193[−1]	1.192[−1]	0.08		30	8.035[−3]	8.035[−3]	0
	10	3.851[−3]	3.849[−3]	0.05		40	1.399[−3]	1.399[−3]	0
	20	4.418[−4]	4.414[−4]	0.09	30	31	6.008	5.980	0.47
	30	1.288[−4]	1.288[−4]	0		40	1.043[−2]	1.043[−2]	0
	40	5.405[−5]	5.402[−5]	0.06	40	41	7.916	7.879	0.47
3	4	8.420[−1]	8.383[−1]	0.44		50	1.279[−2]	1.279[−2[	0
	40	8.474p−5]	8.473[−5]	0.01	50	51	9.824	9.777	0.48
5	6	1.231	1.226	0.41		98	2.522[−4]	2.522[−4]	0
	7	2.070[−1]	2.067[−1]	0.14	100	101	1.936[+1]	1.927[+1]	0.46
	10	2.104[−2]	2.104[−2]	0	200	201	3.844[+1]	3.826[+1]	0.47
	20	1.382[−3]	1.382[−3]	0	400	401	7.660[+1]	7.623[+1]	0.48
	30	3.686[−4]	3.686[−4]	0	700	701	1.338[+2]	1.332[+2]	0.45
	40	1.500[−4]	1.500[−4]	0	900	901	1.720[+2]	1.712[+2]	0.47
						903	7.332	7.330	0.03
						905	1.664	1.644	0

$$g_{\parallel}(n,\varepsilon)\cong 1-\frac{0.172\,826(1-n^2\varepsilon)}{[(1+n^2\varepsilon)n]^{2/3}}-\frac{0.016\,531\,9(3+4n^2\varepsilon+3n^4\varepsilon^2)}{[(1+n^2\varepsilon)n]^{4/3}}+\frac{(1-n^2\varepsilon)(3+4n^2\varepsilon+3n^4\varepsilon^2)}{175[(1+n^2\varepsilon)n]^2}+O(1/n^{8/3})\ ,\quad n^2\varepsilon \ll 1\ . \tag{5}$$

The factor $1-\exp(-2\pi/\sqrt{\varepsilon})$ in (5) is set equal to unity, since for most cases of interest it is close to 1.

Menzel and Pekeris [1] give an asymptotic formula for $g_{\parallel}(n,\varepsilon)$ when $n^2\varepsilon \gg 1$. However, this formula is the same as the formula given for $n^2\varepsilon \ll 1$. This is evident by examining Eqs. (1.39) and (1.40) of their paper, where the first equation applies to the case when $n^2\varepsilon \ll 1$, and the second to the case when $n^2\varepsilon \gg 1$. Their Eq. (1.40) is identical to Eq. (1.39), as is evident by multiplying the numerator and denominator of the second and third terms on the right-hand side of (1.40) by κ^2/n'^2 and κ^4/n'^4, respectively. Equation (1.40) then reduces to (1.39), which is valid for $n^2\varepsilon \ll 1$ only.

Omidvar and Guimaraes [10], after replacing n' by $i/\sqrt{\varepsilon}$, have expanded directly the hypergeometric functions appearing in (2) in terms of $\varepsilon^{-1/2}$. Making use of this expansion, we find that

$$g_{\parallel}(n,\varepsilon)\cong \frac{4\sqrt{3}}{\varepsilon^{1/2}}\left[1-\frac{\pi}{\varepsilon^{1/2}}+\frac{1}{3\varepsilon}(\pi^2+10-5/n^2)-\frac{\pi}{3\varepsilon^{3/2}}(7-2/n^2)+O(1/\varepsilon^2)\right]\ ,\quad n^2\varepsilon \gg 1\ . \tag{6}$$

In Table I, results of the corrected five-term calculation of Menzel and Pekeris [1] and the eight-term calculation of the present work are compared with the exact values of the bound-bound and bound-continuum oscillator strengths. The percentage error is the percentage difference between the exact and the approximate values given by the asymptotic expansion. As is seen, in going from five-term to eight-term expansion, the error percentage is reduced by an order of magnitude.

For the bound-bound oscillator strength $f(n,n')$ in

TABLE III. A comparison of the eight-term approximation of AEA, $g_{\parallel}(n^2\varepsilon \ll 1)$, and the direct expansion approximation, $g_{\parallel}(n^2\varepsilon \gg 1)$, with the exact values of the bound-free Gaunt factor, $g_{\parallel}(n,\varepsilon)$ [5,10]. Numbers in brackets indicate powers of ten.

n	ε (Ry)	$g_{\parallel}(n,\varepsilon)$	$g_{\parallel}(n^2\varepsilon \ll 1)$	$g_{\parallel}(n^2\varepsilon \gg 1)$	Error (%)
1	0.00	7.97[−1]	7.95[−1]		−0.25
	0.01	8.00[−1]	7.97[−1]		−0.38
	0.10	8.22[−1]	8.19[−1]		−0.36
	1.00	9.42[−1]	9.34[−1]		−0.85
	10.00	9.26[−1]	9.37[−1]		+1.19
	20.00	8.21[−1]	7.49[−1]		−8.77
	10[+2]	5.13[−1]		5.06[−1]	−1.36
	10[+3]	1.99[−1]		1.98[−1]	−0.50
	10[+4]	6.71[−2]		6.71[−2]	0.00
2	0.00	8.76[−1]	8.76[−1]		0.00
	1.00	1.05	1.05		0.00
	5.00	1.03	1.05		+1.94
	25.00	7.88[−1]		7.84[−1]	−0.51
	10[+4]	6.72[−2]		6.72[−2]	0.00
5	0.00	9.36[−1]	9.36[−1]		0.00
	1.00	1.09	1.10		+0.92
	16.00	8.75[−1]	8.46[−1]		−3.31
	25.00	7.90[−1]		7.98[−1]	+1.01
	10[+2]	5.15[−1]		5.16[−1]	+0.19
	10[+4]	6.72[−2]		6.72[−2]	0.00
10	0.00	9.61[−1]	9.61[−1]		0.00
	1.00	1.10	1.10		0.00
	16.00	8.75	8.46		−3.31
	25.00	7.90[−1]		8.00[−1]	+1.27
	2.5[+3]	1.30[−1]		1.30[−1]	0.00
20	0	9.76[−1]	9.76[−1]		0.00
	25.00	7.90[−1]		8.01[−1]	+1.39
	2.5[+2]	3.62[−1]		3.62[−1]	0.00
40	0	9.85[−1]	9.85[−1]		0.00
	0.625	1.10	1.10		0.00
50	0	9.87[−1]	9.87[−1]		0.00
	0.04	1.05	1.05		0.00

Table II, comparison of the exact results is made with the results of the asymptotic expansion approximation (AEA). In that table random values of n and n' are chosen, where n and n' range from 1 to 900 and 2 to 905, respectively. The exact values for $n \leq 50$ are due to the numerical integration of Green, Rush, and Chandler [4]. The exact values of $f(n,n')$ for $n > 50$ are due to Menzel [3], who makes use of an infinite expansion of the inverse hypergeometric functions. It is noteworthy that the percentage of errors for all transitions, including the lowest $n = 1$ to $n' = 2$ transition, does not exceed 0.5%, although the validity criterion for the asymptotic expansion approximation dictates $n \gg 1$ and $\alpha = n/n' \ll 1$.

In Table III, the bound-continuum Gaunt factor is considered, and comparison is made between the exact and the approximate values. For the $n^2\varepsilon/\text{Ry} \gg 1$ Ry cases in Table III, Eq. (6), based on a derivation of Omidvar and Guimaraes [10], has been used.

For n values considered in Table III and $\varepsilon \leq 1$ Ry, the AEA values given by (5) are within 1% of the exact values [5,10]. Similarly, for $\varepsilon \geq 100$ Ry, the Gaunt factors based on Eq. (6) are within 1% of the exact values. For 1 Ry $< \varepsilon <$ 100 Ry, numerical integration should be used.

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