PHYSICAL REVIEW A VOLUME 46, NUMBER 9 1 NOVEMBER 1992

Semiclassical description of dipole matrix elements for arbitrary $nl \to n'l'$ transitions in nonhydrogenic ions

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(Received 20 April 1992)

A semiclassical formula for dipole matrix elements of single-electron $nl \to n'l'$ transitions with arbitrary quantum numbers in nonhydrogenic ions is derived. Only the energies and angular momenta of the initial and final states are needed as input along with the charge of the ion. The definition of the intermediate state is a key element in the derivation. Results are compared with experimental values and self-consistent-field calculations for Na-like ions. The formula is shown to coincide with the exact quantum-mechanical result for hydrogen in the limit $n' \gg n \gg 1$, $l \ll n$.

PACS number(s): 31.50.+w, 52.25.−b, 31.15.+q, 31.20.−d

I. INTRODUCTION

In the last decade, new attention has been paid to semiclassical methods for calculating oscillator strengths of atomic $nl \to n'l'$ transitions [1–8]. The present paper, it is hoped, will add another significant step to this development. Besides the use of WKB wave functions, the Coulomb approximation [9–12] provides the basis for a simple treatment of nonhydrogenic states in terms of quantum defects and corresponding phase shifts.

One of the driving forces came from the study of Rydberg states; though exact quantum-mechanical expressions [13] for these almost pure hydrogenic states are available, numerical problems in the evaluation of the hypergeometric functions are encountered for the region of very high quantum numbers, where the semiclassical expressions have no difficulties and become very accurate. A second important motivation stems from laser plasma physics, where one has to cope with huge numbers of transitions in highly perturbed ions and needs efficient tools to calculate radiation coefficients, but can afford lower ($\leq 10\%$) accuracy. The present work was partially stimulated by such plasma applications [7,14].

The semiclassical approach for Rydberg transitions ($n,n' \gg 1$) including quantum defects was developed for $|n'-n| \ll n$ by Davydkin and Zon [2]. Recently, D'yachkov and Pankratov [8] treated bound-state–bound-state, bound-state–free-electron, and free-electron–free-electron nonhydrogenic transitions in the limit $Z\omega/|E|^{3/2} \gg 1$ and $Z\omega/|E'|^{3/2} \gg 1$, where Z is the charge of the ion when the active electron is subtracted, $\omega = E' - E$, and E and E' are the energies of the lower and the upper state; for bound-state–bound-state transitions, it is equivalent to $n' - n \gg 1$ and $n \gg 1$. In this limit, one can set $E = E' = 0$ in the WKB wave functions, corresponding to a parabolic classical orbit. Here and in the following, atomic units are used.

The present paper aims for a generalization, valid for any quantum numbers. Allowing for large differences between E and E', the major achievement in the following will be the definition of a semiclassical state with an energy E_c intermediate between E and E'. It will be characterized by a *stationarity* condition stating that the difference between the phases of the two wave functions integrated over the intermediate orbit must be a multiple of 2π; in addition, E_c must be chosen as close as possible to $(E+E')/2$. Under these conditions, a simple analytic expression for the radial dipole matrix element is obtained, which is shown to reproduce the results in the Rydberg region, mentioned above, and also to coincide with the exact quantum-mechanical result for hydrogen in the limit $n' \gg n \gg 1$ and $l \ll n$. In the last section, we compare the present result with self-consistent-field calculations and experiments for some sample transitions and find excellent agreement.

II. PHASE SHIFTS AND QUANTUM DEFECTS

The radial dipole matrix element is given by

$$D_{nl}^{n'l'} = \int R_{n'l'}(r) R_{nl}(r) r^3 dr \tag{1}$$

with $l' = l \pm 1$ and radial wave functions $R_{nl}(r)$. The basic assumption of the Coulomb approximation [9] is that significant contributions to the integral (1) arise only from regions with relatively large r where the potential $V(r)$ felt by the active electron is well represented by the Coulomb potential Z/r of the ion core with charge $Z = Z_{\text{ion}} - 1$; the ion core, together with the active electron, represents the total ion with charge Z_{ion}. In this region, the semiclassical WKB wave function has the form

$$R_{nl}(r) = \frac{A_{nl}}{r P_{nl}(r)^{1/2}} \cos\Phi_{nl}(r) , \tag{2}$$

with $P_{nl}(r) = [2E_{nl} + 2Z/r - (l+1/2)^2/r^2]^{1/2}$ and

$$\Phi_{nl}(r) = \int_a^r P_{nl}(r) dr + \delta_{nl} - \frac{\pi}{4} . \tag{3}$$

The phase shift δ_{nl} accounts for the difference between $V(r)$ and Z/r in the inner, non-Coulomb region. The classical turning points are given by $P_{nl}(a) = P_{nl}(b) = 0$. By means of the Bohr-Sommerfeld quantization condition

$$\int_a^b P_{nl}(r)dr+\delta_{nl}=\pi(n-l-\tfrac{1}{2}) , \tag{4}$$

the energy is obtained as

$$E_{nl}=-\frac{Z^2}{2\nu_{nl}^2} \tag{5}$$

with the effective quantum number $\nu_{nl}=n-\delta_{nl}/\pi$. The phase shift is directly related to the so-called quantum defect $\mu_{nl}=\delta_{nl}/\pi$. In practice, we shall determine the phase shifts $\delta_{nl}=n-Z/\sqrt{2|E_{nl}|}$ from the energies E_{nl}, which are either taken from experiment or from other calculations.

III. SEMICLASSICAL EXPRESSION FOR DIPOLE MATRIX ELEMENT

In evaluating Eq. (1), the indices nl and $n'l'$ are suppressed; all dashed quantities refer to the upper state. A number of approximate steps is made

$$\begin{aligned}D_{nl}^{n'l'}&=AA'\int_a^b\cos\Phi'(r)\cos\Phi(r)\frac{r\,dr}{[P(r)P'(r)]^{1/2}}\\&\approx\frac{AA'}{2}\int_a^b\cos(\Phi'-\Phi)\frac{r\,dr}{[P(r)P'(r)]^{1/2}}\\&\approx\frac{AA'}{2}\int_{a_c}^{b_c}\cos(\Phi'-\Phi)\frac{r\,dr}{P_c(r)} .\end{aligned} \tag{6}$$

First, a rapidly oscillating term $\cos(\Phi'+\Phi)$ is neglected, and then the product $[P(r)P(r')]^{1/2}$ is replaced by a centered momentum

$$P_c(r)=(2E_c+2Z/r-\lambda_c^2/r^2)^{1/2} \tag{7}$$

with turning points $P_c(a_c)=P_c(b_c)=0$ and $\lambda_c=(l+l'+1)/2$. For large transition energies $\omega=E'-E$, the validity of this latter replacement is far from obvious. A proper choice of the centered energy E_c will be discussed further below. The phase difference in Eq. (6) is transformed to

$$\begin{aligned}\Phi'-\Phi&\approx\int_{a_c}^{r}\frac{P'^2(r')-P^2(r')}{2P_c(r')}dr'+\Delta\delta\\&=\int_{a_c}^{r}\left[E'-E-\Delta\lambda\frac{\lambda_c}{r'^2}\right]\frac{dr'}{P_c(r')}+\Delta\delta ,\end{aligned} \tag{8}$$

where $\Delta\delta=\delta'-\delta$ and $\Delta\lambda=l'-l=\pm1$. The integrations are performed following a standard technique. Equation (8) involves the classical Kepler integrals [15] for time t and azimuthal angle ϕ

$$t=\int_{a_c}^{r}\frac{dr'}{P_c(r')},\quad \phi=\int_{a_c}^{r}\frac{\lambda_c dr'}{r'^2P_c(r')} ,$$

which lead to the parametric representation of the elliptic orbit

$$\begin{aligned}&r=(\nu_c^2/Z)(1-\epsilon\cos\xi) ,\\&t=(\nu_c^3/Z^2)(\xi-\epsilon\sin\xi) ,\\&\cos\phi=(\cos\xi-\epsilon)/(1-\epsilon\cos\xi) ,\\&\sin\phi=(1-\epsilon^2)^{1/2}\sin\xi/(1-\epsilon\cos\xi) ,\end{aligned} \tag{9}$$

with the eccentricity $\epsilon=[1-(\lambda_c/\nu_c)^2]^{1/2}$ and $\nu_c=Z/\sqrt{2|E_c|}$. Inserting Eq. (8) into Eq. (6), we obtain, after some lengthy calculation,

$$\begin{aligned}D_{nl}^{n'l'}&\approx AA'/2\int_0^{T/2}r\cos[\omega t-\Delta\lambda\phi(t)+\Delta\delta]dt\\&=\frac{Z\nu_c^2}{\omega(\nu\nu')^{3/2}}\{U_\gamma(\epsilon\gamma)\cos\Delta\delta-V_\gamma(\epsilon\gamma)\sin\Delta\delta+W_\gamma\} ,\end{aligned} \tag{10}$$

where all energies $E=-Z^2/(2\nu^2)$ are expressed by the corresponding effective quantum numbers ν; the normalization constants are taken as $A^2=2Z^2/(\pi\nu^3)$, $\omega=E'-E$, and $\gamma=\omega\nu_c^3/Z^2$; $T=(2\pi/\omega)\gamma$ is the period of the orbit; and

$$\begin{aligned}U_\gamma(y)&=J'_\gamma(y)+\Delta\lambda\frac{(1-\epsilon)^{1/2}}{\epsilon}J_\gamma(y) ,\\V_\gamma(y)&=E'_\gamma(y)+\Delta\lambda\frac{(1-\epsilon^2)^{1/2}}{\epsilon}\left[E_\gamma(y)-\frac{1}{\pi\gamma}\right]\\&\quad+\frac{(1-\epsilon)}{\pi} ,\\W_\gamma&=-\frac{\sin(\pi\gamma+\delta'-\delta)}{\pi\gamma}\left[(1+\epsilon)\gamma+\Delta\lambda\frac{(1-\epsilon^2)^{1/2}}{\epsilon}\right] ,\end{aligned} \tag{11}$$

with Anger's and Weber's function

$$J_\gamma(y)=\frac{1}{\pi}\int_0^\pi\cos(\gamma\xi-y\sin\xi)d\xi , \tag{12}$$

$$E_\gamma(y)=\frac{1}{\pi}\int_0^\pi\sin(\gamma\xi-y\sin\xi)d\xi , \tag{13}$$

respectively. For integer γ, $J_\gamma(y)$ is identical with the corresponding Bessel function. For noninteger γ, these functions can be calculated [16] from

$$\begin{aligned}J_\gamma(y)&=\frac{\sin\gamma\pi}{\gamma\pi}f_\gamma(y)+\frac{\sin\gamma\pi}{\pi}g_\gamma(y) ,\\E_\gamma(y)&=\frac{1-\cos\gamma\pi}{\gamma\pi}f_\gamma(y)-\frac{1+\cos\gamma\pi}{\pi}g_\gamma(y) ,\end{aligned} \tag{14}$$

with the expansions

$$\begin{aligned}f_\gamma(y)&=1-\frac{y^2}{2^2-\gamma^2}+\frac{y^4}{(2^2-\gamma^2)(4^2-\gamma^2)}\\&\quad-\frac{y^6}{(2^2-\gamma^2)(4^2-\gamma^2)(6^2-\gamma^2)}+\cdots ,\\g_\gamma(y)&=\frac{y}{1^2-\gamma^2}-\frac{y^3}{(1^2-\gamma^2)(3^2-\gamma^2)}+\cdots ,\end{aligned} \tag{15}$$

and the derivatives are given by $J'_\gamma(y)=[J_{\gamma-1}(y)-J_{\gamma+1}(y)]/2$ and $E'_\gamma(y)=[E_{\gamma-1}(y)-E_{\gamma+1}(y)]/2$.

IV. OPTIMAL INTERMEDIATE STATE

The crucial question still to be answered is how to choose the intermediate state. It was introduced in Eq. (6). First its energy E_c has to be selected; the momentum $P_c(r)$ and the turning points a_c and b_c are then given according to Eq. (7). We find that two conditions have to be fulfilled.

(i) The intermediate state has to be *stationary* in the sense that the phase difference, given by Eq. (8),

$$\int_{a_c}^{b_c} \left[E' - E - \Delta\lambda \frac{\lambda_c}{r'^2} \right] \frac{dr'}{P_c(r')} + \Delta\delta = \pi\gamma \pm \pi + \Delta\delta = \pi N \tag{16}$$

is a multiple of π when extended over the full radial interval from a_c to b_c. This condition guarantees that the term W_γ, defined by Eq. (11), becomes identically zero. It is required to recover well-known limiting cases from Eq. (10), as we shall show below.

(ii) The integer N in Eq. (16) has to be chosen such that E_c is as close as possible to $(E'+E)/2$. This leads to the condition

$$\gamma = \frac{\omega \nu_c^3}{Z^2} = \left\langle \frac{\omega Z}{|E'+E|^{3/2}} - \Delta\nu \right\rangle + \Delta\nu \ , \tag{17}$$

where $\langle\ \rangle$ denotes the closest integer, and $\Delta\nu = \nu' - \nu$.

With this choice for γ and ν_c, we obtain

$$D_{nl}^{n'l'} = \frac{Z\nu_c^2}{\omega(\nu\nu')^{3/2}} [U_\gamma(\epsilon\gamma)\cos(\pi\Delta\nu) - V_\gamma(\epsilon\gamma)\sin(\pi\Delta\nu)] \ . \tag{18}$$

This is the central result of the present paper. It represents the radial dipole matrix element as a simple analytic function of the energies $E = -Z^2/2\nu^2$, $E' = -Z^2/2\nu'^2$, the angular momenta l and l', and the charge $Z = Z_{\text{ion}} - 1$ of the ion core. Recall that $\omega = E' - E$, $\epsilon = [1 - (l + l' + 1)^2/(2\nu_c)^2]^{1/2}$, $\Delta\nu = \nu' - \nu$, and that the functions U_γ and V_γ are defined in Eq. (11). The essential difference between Eq. (18) and the results obtained previously by other authors [2,3,5,8] lies in the particular choice of ν_c.

V. ASYMPTOTIC LIMITS

The choices made above concerning the intermediate state are now justified by considering asymptotic limits and comparing with known quantum-mechanical and classical results. No agreement is found, unless $W_\gamma \equiv 0$; therefore the *stationarity* condition in Eq. (15) has to be required.

The important asymptotic limit is $\gamma \gg 1$ and $\lambda_c/\nu_c \ll 1$, equivalent to $|1-\epsilon| \ll 1$. In this case, the leading terms in the asymptotic expansion

$$\begin{aligned} J_\gamma(\epsilon\gamma) &\approx (2/\gamma)^{1/3}\text{Ai}(x) \ , \\ J'_\gamma(\epsilon\gamma) &\approx -(2/\gamma)^{2/3}\text{Ai}'(x) \ , \\ E_\gamma(\epsilon\gamma) &\approx (2/\gamma)^{1/3}\text{Gi}(x) \ , \\ E'_\gamma(\epsilon\gamma) &\approx -(2/\gamma)^{2/3}\text{Gi}'(x) \ , \end{aligned} \tag{19}$$

with $x \approx 2^{1/3}\gamma^{2/3}(1-\epsilon) \approx (\omega\lambda_c^3/2Z^2)^{2/3}$ can be obtained from the corresponding integral representations in Eqs. (12) and (13); they are used in Eq. (18) and give

$$D_{nl}^{n'l'} = \frac{2^{2/3}}{Z(\nu\nu')^{3/2}} \left[\frac{Z^2}{\omega} \right]^{5/3} [S(x)\cos\Delta\delta - T(x)\sin\Delta\delta] \tag{20}$$

with

$$\begin{aligned} S(x) &= -\text{Ai}'(x) + \Delta\lambda x^{1/2}\text{Ai}(x) \ , \\ T(x) &= -\text{Gi}'(x) + \Delta\lambda x^{1/2}\text{Gi}(x) + \frac{x}{2\pi} \ , \end{aligned} \tag{21}$$

where Ai(x) and Gi(x) are Airy and Airy-Hardy functions, respectively. This formula was derived before by D'yachkov and Pankratov [8]. It is found here under the condition $W_\gamma \equiv 0$; no condition is obtained concerning E_c, since the corresponding ν_c is dropping out in this limit.

A more subtle check can be made by comparing with the exact quantum-mechanical result for hydrogen, first derived by Gordon [13]. In the limit $n' \gg n \gg 1$ and $l \ll n$, Burgess [17] succeeded to reduce Gordon's formula to the form

$$\begin{aligned} D_{nl}^{n'l+1} = 1.3044 &\left[\frac{(n'+l+1)!(n-l-1)!}{(n'-l-2)!(n+l)!} \right]^{1/2} \\ &\times \left[\frac{n}{n'} \right]^{l+3} \frac{1}{n^{2/3}[1-(n/n')^2]^{5/3}} \\ &\times \left[1 + 0.1788 \frac{(5l+4)-(n/n')^2(5l+6)}{n^{2/3}[1-(n/n')^2]^{2/3}} \right. \\ &\left. + O\left[\frac{1}{n} \right] \right] . \end{aligned} \tag{22}$$

For comparison, one should notice that $\delta' = \delta = 0$, $\nu = n$, $\nu' = n'$ for hydrogen, and that γ becomes an integer due to Eq. (17). Therefore Eq. (18) reduces to

$$D_{nl}^{n'l'} = \frac{Z\nu_c^2}{\omega(nn')^{3/2}} \left[J'_\gamma(\epsilon\gamma) + \Delta\lambda \frac{(1-\epsilon^2)^{1/2}}{\epsilon} J_\gamma(\epsilon\gamma) \right] , \tag{23}$$

where J_γ now denote Bessel functions with integer index. In the region $1 \ll \gamma \ll (\nu_c/\lambda_c)^2$, considered here, the asymptotic expansion of Bessel functions [18] in powers of $\gamma^{-1/3}$ leads to

$$\begin{aligned} D_{nl}^{n'l'} = \frac{Z\nu_c^2}{\omega(nn')^{3/2}} &\left[-\left[\frac{2}{\gamma} \right]^{2/3} \text{Ai}'(0) - \left[\frac{2}{\gamma} \right]^{4/3} \frac{\text{Ai}(0)}{10} \right. \\ &\left. + \Delta\lambda \left[\frac{\lambda_c}{\nu_c} \right] \left[\frac{2}{\gamma} \right]^{1/3} \text{Ai}(0) + \cdots \right] , \end{aligned} \tag{24}$$

where the Airy functions Ai(x) with $x \approx 2^{1/3}\gamma^{2/3}(1-\epsilon) \ll 1$ were also expanded in powers of x. It is found that the second and third term in Eq. (24) can be of same order, but all successive terms are smaller and are neglected. The second term proportional to $(2/\gamma)^{4/3}$ retains a $1/\nu_c^2$ dependence and is sensitive to the choice of E_c. Choosing $E_c \approx (E'+E)/2$, we have $1/\nu_c^2 \approx [1+(n/n')^2]/2n^2$, $\gamma = \omega \nu_c^3/Z^2$, $\omega/Z^2 = [1-(n/n')^2]/(2n^2)$ and specializing to $\Delta\lambda = l'-l = +1$ and $Z=1$, we obtain

$$D_{nl}^{n'l+1} = \frac{2^{7/3}(nn')^{11/6}}{(n'^2-n^2)^{5/3}} \times \left[-\mathrm{Ai}'(0) + \frac{\mathrm{Ai}(0)}{2^{2/3}5} \frac{(5l+4)-(n/n')^2(5l+6)}{n^{2/3}[1-(n/n')^2]^{2/3}} + O\left[\frac{1}{n}\right]\right] . \quad (25)$$

Taking into account $(n+k)! \approx \sqrt{2\pi} n^{n+k+1/2} \exp(-n)$ for $|k| \ll n$, $\mathrm{Ai}(0) = 0.355\,02$ and $\mathrm{Ai}'(0) = -0.258\,82$ [18], we find Eqs. (22) and (25) to be identical. This is a remarkable result. It depends on $E_c \approx (E'+E)/2$; apparently, this is the best possible choice for E_c.

In the limit $n \gg 1$ and $|n'-n| \ll n$, corresponding to small values of γ, it is easy to show that Eq. (18) leads to the classical result for the radiation emission of an electron on an elliptical orbit (see, e.g., Ref. [19]), in agreement with the correspondence principle. Here, we give no explicit derivation, since one gains no additional information concerning E_c.

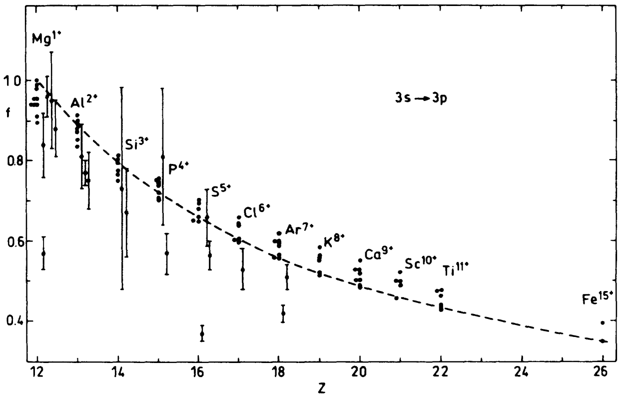

FIG. 1. Oscillator strengths $f_{3s\rightarrow 3p}$ in Na-like ions. Results obtained with Eq. (18) (dashed lines) are compared with experimental data and calculations (dots) from Ganas [21].

VI. COMPARISON WITH EXPERIMENT AND OTHER CALCULATIONS

Turning to the numerical values, the important practical observation is that oscillator strengths based on Eq. (18) agree remarkably well with experimental results and self-consistent-field calculations. Results are compared in Figs. 1 and 2 for $3s \rightarrow 3p$ and $3s \rightarrow 4p$ transitions in Na-like ions from Mg to Fe. The input energies, needed to determine the quantum defects, were also calculated semiclassically [20]. Oscillator strengths

$$f_{nl\rightarrow n'l+1} = \tfrac{2}{3}[(l+1)/(2l+1)]\omega |D_{nl}^{n'l+1}|^2 \quad (26)$$

are plotted. The experimental values with error bars and the theoretical points (Hartree-Fock, pseudopotential,

TABLE I. Radial dipole matrix elements for hydrogen in atomic units. Results from Eq. (18) and from Ref. [7] are compared with exact quantum-mechanical values.

Transition	$D_{nl}^{n'l'}$ Eq. (18)	$D_{nl}^{n'l'}$ Exact	Difference (%) Eq. (18)↔Exact	Difference (%) More [6]↔Exact
1s-2p	1.364	1.290	5.70	3.04
1s-3p	0.584	0.517	13.1	4.45
1s-4p	0.352	0.305	15.6	8.21
1s-5p	0.244	0.209	16.8	8.49
2s-3p	3.119	3.065	1.77	2.58
2p-3d	4.843	4.748	2.00	2.86
2p-3s	0.975	0.938	3.86	6.76
3s-4p	5.517	5.469	0.88	4.97
3p-4d	7.635	7.565	0.93	0.85
3p-4s	2.477	2.443	1.37	10.42
3d-4f	10.34	10.23	1.03	2.98
3d-4p	1.354	1.302	3.98	10.41
10s-11p	40.47	40.43	0.10	8.74
10s-20p	1.791	1.787	0.21	4.25
10s-40p	0.446	0.446	0.02	3.65
10l-40m	0.130	0.121	6.74	9.62
10k-40l	0.255	0.257	0.77	5.76
10h-40i	0.583	0.584	0.14	5.56
10h-20i	2.506	2.512	0.26	4.46
10d-20f	2.296	2.292	0.18	3.02
10i-11j	78.09	78.01	0.10	0.61
10d-11f	51.14	51.09	0.10	6.11

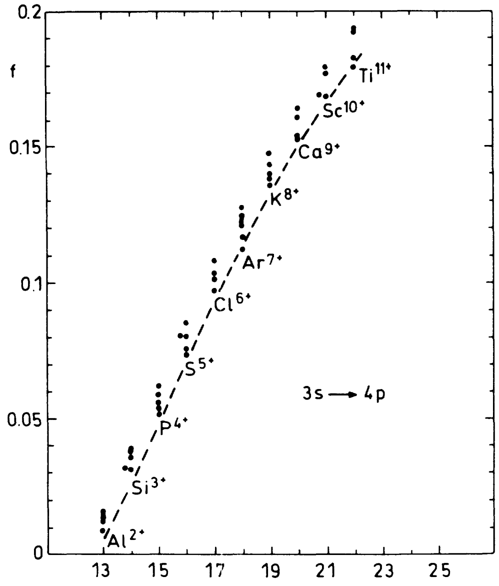

FIG. 2. Oscillator strengths $f_{3s\rightarrow 4p}$ in Na-like ions. Results obtained with Eq. (18) (dashed line) are compared with calculations (dots) from Ganas [21].

semiempirical and other approaches) are taken from Ref. [21]. It is seen that the present results reproduce the variation of the oscillator strength within the isoelectronic series very well, not only for the strong $3s \rightarrow 3p$ transitions, but also for the $3s \rightarrow 4p$ transitions with the characteristic suppression close to aluminum.

A comparison with exact quantum-mechanical matrix elements for hydrogen is given in Table I. Exact hydrogen energies having no quantum defects were used as input in Eq. (18). The differences between semiclassical and exact results are typically 1% and smaller, except for transitions involving states with radial quantum number $n_r = n - l - 1 = 0$. These circular orbits, which have maximum angular momentum and no radial nodes, play a special role in the semiclassical theory, and alternative analytic expressions have been proposed [6] for the nonhydrogenic case. For K-shell transitions, showing the largest deviations in Table I, simple expressions can be obtained when using exact $1s$ wave functions for the lower state.

In Table I, we also compare with recent results of More and Warren [7], who used a different kind of semiclassical approach. Except for transitions with $n_r = 0$ states, the results of the present paper are more accurate, especially for states with higher quantum numbers.

VII. CONCLUSIONS

A simple analytic expression for radial matrix elements for $nl \rightarrow n'l'$ transitions in nonhydrogenic ions has been derived. It extends the applicability of the semiclassical approach to transitions with small n, n' and also allows for large differences $n' - n$. It does not require one to know the atomic potential, but depends only on the energies and the angular momenta of the lower and upper state and the charge of the ion. It is proposed that it be used instead of time-consuming Hartree-Fock calculations, e.g., in the context of dense plasma calculations where one needs many of these matrix elements for determining radiation coefficients and other properties.

The present result applies to low- and medium-Z elements; for high-Z elements, a relativistic generalization has to be worked out. The comparison with some experimental values and with results of self-consistent-field calculations, made in this paper, is promising. However, a systematic comparison with Hartree-Fock calculations covering a larger region of transitions, ionization stages, and elements has still to be performed.

ACKNOWLEDGMENTS

One of the authors (P.P.) wants to thank Dr. S. Witkowski for the hospitality he enjoyed at the Max-Planck-Institut für Quantenoptik. The authors thank Dr. M. Basko for carefully reading the manuscript. This work was supported in part by the Bundesminister für Forschung und Technologie (Bonn, FRG) and by EURATOM.

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