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Energy levels and the oscillator strengths of the Be atom determined by a configuration-interaction calculation with a finite basis set from *B* splines

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The simple configuration-interaction calculational procedure for an alkaline-earth atom is extended to include the *continuum* contribution to the Hamiltonian matrix evaluated in a basis set constructed from a *quasicomplete* set of discrete one-particle orbitals expanded in terms of a set of B splines. The procedure is successfully applied to the study of the energy eigenvalues, the excitation energies, and the oscillator strengths for transitions between selected $^{1,3}S$, $^{1,3}P$, and $^{1,3}D$ states of the beryllium atom. In addition to the simplicity of this calculational procedure and its effectiveness in generating atomic spectroscopy data for an extended spectral region in a *single* calculation with a single basis set, our numerical results have shown that the quantitative *reliability* of this procedure is comparable to or better than many other more elaborate theoretical approaches.

I. INTRODUCTION

The recent advancement of high-resolution intense lasers in the uv region has opened up new experimental possibilities for a more comprehensive study of atomic transitions involving excited states of different symmetry in a complex many-electron atom with a multistep multiphoton process.[1] In contrast to the use of a conventional light source, when a high-power laser is used, even the weak transitions between excited states could contribute significantly in the excitation or the eventual ionization of the atomic electrons. The optimum excitation or ionization "path" in such a process could be chosen more judiciously if a *reliable* theoretical estimation of transition rates between various excited states were available. As lasers of wavelengths in the range of a few hundred nanometers become readily available, the alkaline-earth atoms, with ionization energy ranging approximately from 40 000 to 75 000 cm^{-1}, become particularly attractive for detailed spectroscopic studies. Typically, the alkaline-earth atoms can be ionized or selectively excited to doubly excited autoionization states following the absorption of a small number of photons in the wavelength range of a few hundred nanometers.[1] The spectra of the alkaline-earth atoms below the ionization threshold are relatively simple, although the energy values and oscillator strengths are often affected significantly by configuration mixing from the doubly excited states.[2] In addition, the presence of a large number of doubly excited autoionization states above the ionization threshold makes the alkaline-earth atom an ideal atomic system for a systematic study of *many-electron dynamics*.

As a result of our recent attempt to carry out a comprehensive study on the effect of the multielectron interaction in a complex atom, we have reported in a series of papers[2-6] the quantitative calculations for Mg and its isoelectronic sequence on the term values, the fine-structure level splittings, the oscillator strengths for transitions between states below the first ionization threshold, the position and width of the doubly excited autoionization states above the ionization threshold, and the photoionization dominated by those doubly excited states. The basic theoretical approach employed in our study follows a simple configuration-interaction (CI) calculational procedure outlined earlier.[2-6] For the bound states below the ionization threshold, we have chosen the basis set constructed from the one-particle Hartree-Fock *bound* orbits subject to a potential corresponding to the ^1S frozen core given explicitly in Ref. 3. For the doubly excited autoionization states above the ionization threshold, the basis set is expanded to include the *positive* energy orbits subject to a *screening* potential corresponding to the ionization channel following a modified Fano procedure.[4,7]

In spite of the quantitative success of these calculations, the use of *incomplete bound* basis set for the bound states below the ionization threshold or for the bound component of the autoionization states above the threshold has inevitably left out the possible contribution from the *continuum* component which in principle should also be included as a part of the *complete* basis set constructed from the one-particle orbits generated in the ^1S frozen-core Hartree-Fock Hamiltonian. It is the main purpose of this paper to introduce the use of a *quasicomplete* finite basis set constructed from B splines[8] to replace the incomplete basis set employed in our previous calculations. This finite basis set is constructed from a set of discrete orbits subject to the same frozen-core Hartree-Fock (FCHF) potential. Each orbit represents a discretized eigenfunction of the one-particle FCHF Hamiltonian in a volume of chosen radius and is constructed as a linear combination of B splines confined in this volume. This *quasicomplete* basis set becomes a *complete* set in the limit when the numbers of B splines included in the expansion and the size of the chosen volume both approach infinity.

The effectiveness of the finite basis set constructed from B splines has already been demonstrated in the recent relativistic many-body perturbation calculation.[9] Unlike the Slater-type orbits extensively employed in the construction of finite basis set in many other calculations,[10] the use of *B* splines does not require the procedure of selecting the parameters in the exponential functions. In addition, the bell shape of the *B* splines with similar amplitude tends to treat the entire physical region in the chosen finite volume more uniformly than the Slater-type orbits. Many of the basic properties of *B* splines are discussed in detail elsewhere[8,9,11] and we will limit our discussion to those related to the construction of the nonrelativistic *B* spline basis set in Sec. II.

In Sec. III we will report the result of the first detail numerical application of a simple configuration interaction (CI) calculation with finite basis set constructed from *B* splines to the spectra of Be below the first ionization threshold. Beryllium is perhaps the most extensively studied alkaline-earth atom and many of the most elaborate theoretical approaches in atomic structure calculation have been applied to Be in the past two decades. With an accuracy comparable to or better than most of the existing theoretical approaches in the calculated term values, excitation energies, and oscillator strengths, our numerical results will firmly establish this simple CI procedure as an effective approach in generating *reliable* quantitative spectroscopy data for an *extended* spectral region in a *single* calculation.

The early close-coupling calculation by Norcross and Seaton[12] on the term values of ${}^{1,3}S$ to ${}^{1,3}F$ series, which agree closely with the observed experimental data,[13] has established the quantitative standard for any theoretical calculation on the energy levels for Be atom. In fact, other than the present calculation, only in the most recent multiconfiguration Hartree-Fock (MCHF) calculation by Froese Fischer and her co-worker[14] and the earlier variational superposition-of-configuration (SOC) calculation by Weiss,[15] are the calculated term values comparable or slightly higher in accuracy than that of the close-coupling results. The quantitative accuracy of the theoretical atomic structure calculation can also be measured by the accuracy of the calculated excitation energy for transitions between energy eigenstates. The calculated excitation energies from most of the early CI calculations, including works by Hibbert,[16] Sims and Whitten,[17] and Weiss,[15] are generally in close agreement with the observed data. In addition, in a very sophisticated application of a hierarchy of variational Bethe-Goldstone equations, Moser *et al.*[18] have examined in detail the effect of the electronic correlation and relaxation to the transitions between a few highly correlated states in Be. The requirement of elaborate optimum procedure consistently applied to each of the states involved in the transition and the lack of high speed modern computer in the mid 1970s have unfortunately limited the more extensive application of these potentially effective approaches. Other theoretical approaches, with emphasis given to the transition itself instead of the individual initial and final states, include the multiconfiguration relativistic random-phase approximation (MCRRPA),[19] the first-order theory of oscillator strengths (FOTOS),[20] the relativistic random-phase approximation (RRPA),[21] the nonrelativistic random-phase approximation (RPA)[22] or the equivalent time-dependent Hartree-Fock (TDHF) approximation,[23] and the many-body perturbation calculation (MBPT).[24] Most of these calculations have achieved various degree of quantitative success. One of the most interesting features in some of these calculations is the gauge invariance which assures the agreement of the calculated oscillator strengths in length and velocity approximations.[19,21,22] It is generally accepted that the agreement between the calculated oscillator strengths in length and velocity approximations *alone* should not be taken as a measure of quantitative accuracy. And a more acceptable criterion of quantitative accuracy would require the convergence of the oscillator strengths as more contributing terms are included in the calculation of the transition amplitude in addition to the convergence of the calculated excitation energy to the observed value. On the other hand, it should also be emphasized that the agreement between length and velocity results should *not* be disregarded as a critical test in establishing the quantitative reliability of any viable theoretical approach.

In a simple CI calculation the eigenstates are usually represented by a linear combination of a predetermined basis set without the optimization procedure required for each individual state as in a more elaborate CI calculation. The absence of the variational requirement for each state and the use of a single basis set make it possible to calculate the energy eigenvalues and the oscillator strengths for an extended spectral region in a *single* calculation. One of such approaches is the model potential calculation by Laughlin and Victor and their co-workers.[25] The model potential calculation is similar to our recent CI calculation except in the size of the basis set and few minor computational details. As we have pointed out earlier, the main difficulty in the CI calculation with predetermined basis set is the lack of *continuum* contribution in the *incomplete* basis set. For small atom such as Be, in spite of this theoretical difficulty, the general agreement between all the calculated energy levels and the oscillator strengths in the model potential calculation and the observed data is remarkably good and only slightly worse than the most elaborate calculations. The large-scale simple CI calculation based on the application of the Hartree-Fock-relativistic (HFR) code developed by Cowan[26] has also been carried out for Be by Fawcett.[27] As reported by Fawcett, to optimize the fitting of the calculated transition energies to the observed values for most of the transitions included in the calculation, it is necessary to reduce the direct and exchange Slater radial Coulomb integrals by 90% and 85%, respectively. For the strongly correlated $2p^2$ and $2snd$ ${}^1D$ states, the optimization has failed to reproduce the correct energies even with the adjustment to the Slater integrals.

The combined hyperspherical and eigenchannel *R*-matrix technique and the subsequent combined multichannel quantum-defect theory (MQDT) and eigenchannel *R*-matrix method[28] offer an alternative general approach in the study of the multielectron interaction in alkaline-earth atoms. Recent application of this approach[29] has demonstrated its capability of global interpretation of the complex spectra. Its earlier application to Be with a smaller basis set,[28] however, has failed to achieve the quantitative accuracy comparable to other calculations discussed earlier. In principle, its numerical accuracy should improve significantly if an enlarged basis set is included in the calculation. A more recent rotor-vibrator (RV) approach suggested by Hunter and Berry[30] offers an alternative angular correlation treatment which differs in its calculational procedure from the well-established approach in the standard CI calculation. The calculated oscillator strengths for selected transitions in Be from the RV approach, though compared better than the results from the single-configuration Hartree-Fock approximation, are noticeably different from most of the existing calculations. Detailed comparison for the calculated oscillator strengths, the excitation energies, and the energy eigenvalues from various calculations and available experimental data will be presented in Sec. III.

II. THEORETICAL PROCEDURE

The basic theoretical approach employed in the present work is similar to the simple configuration interaction (CI) calculational procedure outlined in our recent papers.[2-4] The Hamiltonian matrix corresponding to a total spin S and total orbital angular momentum L is calculated with a basis set consisting of a number of configuration wave functions $\Psi^{SL}_{n_il_i,n_jl_j}$ representing the electronic configuration (n_il_i,n_jl_j) for the two valence electrons. The configuration wave function Ψ is given by the sum of Slater determinant wave functions ϕ over the allowed magnetic quantum numbers in the LS coupling. The Slater determinant wave function ϕ is constructed from the one-particle orbit wave function $u_{nlmm_s}(\mathbf{r})$ which is usually the eigenfunction of an effective one-electron Hamiltonian. The angular and the spin part of the one-particle orbital wave function are given by the spherical harmonics Y_{lm} and spin function σ_{m_s}, respectively. The energy eigenvalue and the state wave function Φ of an energy eigenstate are then determined by diagonalizing the Hamiltonian matrix. All simple CI calculations for a quasi-two-electron atom with two electrons outside a ^1S frozen core are carried out essentially with this same procedure. Following this simple CI procedure, the only component in the basis set that is not completely fixed is the radial part χ_{nl} of the one-particle orbital wave function. Therefore, the success of any simple CI calculation depends primarily on the choice of the radial function χ and the size of the basis set included in the calculation of the Hamiltonian matrix.

In most of our recent calculations, the radial function χ satisfies the eigenequation, i.e.,

$$h_l^{\mathrm{HF}}(r)\chi_{nl}(r)=\varepsilon_{nl}\chi_{nl}(r) \ , \tag{1}$$

where h_l^{HF} is the one-particle frozen-core Hartree-Fock (FCHF) Hamiltonian defined explicitly by Eq. (7) in Ref. 3. More specifically, the basis set consists of a number of two-electron *configuration series nll′*. Each configuration series consists of a series of configuration wave functions Ψ corresponding to one electron in a fixed orbital nl and the other electron with fixed orbital angular momentum l' but variable energy eigenvalues. As we pointed out in Sec. I, the configuration series included in all our previous calculation are *incomplete* in that only the bound eigenfunctions $\chi_{n'l'}$ of Eq. (1) corresponding to the negative-energy eigenvalue $\varepsilon_{n'l'}$ are included in each configuration series nll'. To include the contribution from the *continuum* corresponding to the positive-energy eigenfunctions in the configuration series nll', we replace the set of bound only solutions $\chi_{n'l'}$ by an entire set of discrete solutions χ_ν of Eq. (1) constructed from B splines.

To calculate this *quasicomplete* set of solutions χ_ν of Eq. (1), we first rewrite the Eq. (1) into a simpler form

$$-\frac{1}{2}\frac{d^2\chi}{d^2r}+V(r)\chi(r)=\varepsilon\chi(r) \ , \tag{2}$$

where the interaction $V(r)$ is nonlocal in general. The solution χ is expanded in terms of a set of B splines[8,9] of order k and total number n defined between two endpoints $r_{\min}=0$ and $r_{\max}=R$, i.e.,

$$\chi(r)=\sum_{i=1}^{n} c_iB_i(r) \ . \tag{3}$$

The n and k are omitted from the functions B_i for simplicity. Similar to the relativistic calculation by Johnson *et al.*,[9] an exponential knot sequence is used in the present calculation. At the endpoints $r=0$ and $r=R$, all B splines are equal to zero except B_1 and B_n, i.e.,

$$\begin{aligned} &B_1(r=0)=1 \quad \text{and} \quad B_i(r=0)=0, \quad i=2,3,\ldots,n \ ; \\ &B_n(r=R)=1 \quad \text{and} \quad B_i(r=R)=0, \quad i=1,2,\ldots,n-1 \ . \end{aligned} \tag{4}$$

The boundary conditions $\chi(0)=\chi(R)=0$ therefore require that

$$c_1=c_n=0 \ . \tag{5}$$

Substitution of Eqs. (3) and (5) into Eq. (2) leads to a $(n-2)\times(n-2)$ symmetric generalized eigenvalue equation

$$HC=\varepsilon AC \ , \tag{6}$$

where H and A are $(n-2)\times(n-2)$ symmetric matrices given by

$$H_{ij}=-\tfrac{1}{2}\langle B_i|d^2/dr^2|B_j\rangle+\langle B_i|V|B_j\rangle \ , \quad i \text{ and } j=2 \text{ to } n-1 \ ; \tag{7}$$

$$A_{ij}=\langle B_i|B_j\rangle, \quad i \text{ and } j=2 \text{ to } n-1 \ . \tag{8}$$

The eigenfunction χ_ν corresponding to the energy eigenvalue ε_ν is given by

$$\chi_\nu=\sum_{i=2}^{n-1} c_iB_i(r) \ , \tag{9}$$

where the set of $n-2$ coefficients c_i forms the eigenvector

$$C_\nu=(c_2,c_3,\ldots,c_{n-1}) \tag{10}$$

corresponding to ε_v. As expected, the calculated ε_v of the first few lowest negative-energy solutions with their eigenfunctions completely confined in R agree with the numerical solutions of Eq. (1) to 10^{-7} Ry. The set of $n-2$ radial eigenfunctions χ_v of h_l^{HF} constructed from B splines are then used to form the configuration wave functions for each configuration series.

The B splines in the present calculation are confined in a fixed radius R. The value of R is chosen so that it is sufficiently large to cover the estimated physical size of the excited states of our interest. For example, in the present calculation, we have selected $R=150a_0$ to ensure the *reliability* of our calculation for the first four to five excited states in each SL series. The accuracy of our numerical calculation is tested by changing the values of R, n, and k which characterize the B splines set. The first seven figures (i.e., up to 10^{-6} Ry) of the energy eigenvalues of the excited states remain unchanged in our calculation when we vary the value of R from $130a_0$ to $160a_0$. In addition, we have also varied the value of n from 27 to 42 and the value of k from 7 to 9 and, again, the first seven figures of the calculated energy eigenvalues remain unchanged. After selecting $R=150a_0$, $n=27$, and $k=7$ in the present calculation, we then examine the variation of the energy eigenvalues as we increase the size of the basis set. The energy eigenvalue converges rapidly to 10^{-3} Ry when the number of contributing configuration series in the basis set increases from one to about five. To achieve a convergence up to 10^{-4} Ry or better, it will require typically 15 to even higher numbers of configuration series.

In addition to the introduction of a *finite quasicomplete* set of one-particle radial eigenfunctions in the construction of the basis set, a minor modification is included in the present calculation to take into account effectively the interaction between the inner-shell and outer-shell electrons. Similar to our earlier works,[2-6] the interaction between the inner and outer electrons are approximated by adding to the nonrelativistic Hamiltonian two effective interactions V_p and V_d where

$$V_p=\sum_{i=1}^{N} V_s(r_i)-V_\alpha(r_i)\ , \tag{11}$$

$$V_d=-2\sum_{\substack{i,j\\(i\neq j)}}^{N}(\hat{\mathbf{r}}_i\cdot\hat{\mathbf{r}}_j)[V_\alpha(r_i)V_\alpha(r_j)]^{1/2}\ , \tag{12}$$

$$V_\alpha=\frac{\alpha}{r^4}\left(1-e^{-(r/r_0)^6}\right)\ , \tag{13}$$

and

$$V_s=(a_0+a_1r+a_2r^2)e^{-\beta_1 r}+(b_0+b_1r+b_2r^2)e^{-\beta_2 r}\ . \tag{14}$$

The dipole-polarization interaction V_α and the dielectronic interaction V_d are represented by the same expressions employed in our recent calculations. The short-range interaction V_s, in a form similar to the one employed in the model potential calculation by Victor and Laughlin,[25] is added to facilitate the numerical fitting to the correct limits of the singly excited nl series of Be II. In the present calculation the parameters r_0, β_i, a_i, and b_i are fitted so that the energy correction

$$\Delta_{nl}=-\langle\chi_{nl}|V_p|\chi_{nl}\rangle \tag{15}$$

for the first ten singly excited states of Be II are within 1–2 % (i.e., 10^{-4} Ry or less) of the *difference* between the calculated ϵ_{nl} and the experimental limit. Similar to other earlier calculations,[12] we have used the value $\alpha=0.051\,23$ a.u. for the Be III core static polarizability.[31] By separating the inner-shell interactions from the one-particle effective potential in the generation of the radial eigenfunctions χ, the effect of inner-shell interactions can be estimated quantitatively by comparing the numerical results following the diagonalization of the Hamiltonian matrix with and without the contributions from V_p and V_d.

The theoretical procedure for the oscillator strength calculation has been outlined in our recent publication.[2] We have also examined the convergence pattern of the calculated oscillator strengths reported in Sec. III following the similar procedure described earlier.[2] With the radial one-particle eigenfunctions confined in a finite volume, our calculation has shown that the length results have consistently exhibited a more smooth convergence pattern (with a fluctuation of less than 0.1%) than the velocity results (with a fluctuation of less than 1%) as we increase the number of configuration series in our basis set.

III. RESULTS AND DISCUSSIONS

Table I compares the calculated quantum defects for the $2snp\ ^1P$ series converging to the Be II $2s$ limit to the measured values. The calculated quantum defects from the present calculation with B-spline basis set compares very well with the experimental data[13] at an accuracy comparable to or better than the most accurate result from MCHF calculation by Saha and Froese Fischer,[14] the close-coupling calculation by Norcross and Seaton,[12] and the SOC calculation by Weiss.[15] The contribution from the *continuum* component to the quantum defects is significant and can be measured by the difference between the B-spline (B-spline FCHF) result and that calculated with the incomplete bound basis set (bound FCHF). The quantum defects from the model potential calculation by Laughlin and Victor[25] should increase to the bound FCHF values if their basis set is enlarged. The CI result by Hibbert[16] and the R-matrix result by O'Mahony and Greene[28] should also improve if the basis set is expanded in the calculation. Other simple CI calculations by Serrao,[32] using an angular-momentum-dependent scaling Thomas-Fermi-Dirac model potential, and by Markewicz *et al.*,[33] using a combined l-dependent core polarization potential and the frozen-core HF potential fitted to the lowest-energy eigenstate for each excitation series, have yielded quantum-defect values noticeably less accurate than those from other calculations.

The quantum defects for the strongly correlated $2p^2$ and $2snd\ ^1D$ series converging to the Be II $2s$ limits are listed in Table II. Again, the accuracy of the calculation can be determined by measuring the calculated quantum

TABLE I. Quantum defects for $2snp\ ^1P$ series converging to Be II $2s$ limits. The present (B-spline FCHF) result represents the CI calculations with set of the B-spline basis set subject to the ^1S frozen-core Hartree-Fock potential. The present (bound FCHF) result represents the CI calculations with basis set including only the bound orbits subject to the ^1S frozen-core Hartree-Fock potential.

Theory	$2s2p$	$2s3p$	$2s4p$	$2s5p$	$2s6p$
Present (B-spline FCHF)	0.1569	0.2888	0.3274	0.3451	0.3554
Present (bound FCHF)	0.1262	0.2533	0.2949	0.3145	0.3260
Saha and Froese Fischer[a]	0.1582				
Norcross and Seaton[b]	0.1506	0.2834	0.3226	0.3405	0.3505
Weiss[c]	0.1504	0.2715	0.3104		
Hibbert[d]	0.1481				
Laughlin and Victor[e]	0.1182	0.2413	0.2804	0.2877	0.2874
O'Mahony and Greene[f]	0.085	0.235	0.319		
Serrao[g]	0.0265	0.1889	0.2588	0.2936	
Markiewicz *et al.*[h]	0.1661[i]	0.1713	0.1753	0.1776	0.1797
Observed[j]	0.1661	0.2958	0.3324	0.3487	0.3574

[a] Reference 14.
[b] Reference 12.
[c] Reference 15.
[d] Reference 16.
[e] Reference 25.
[f] Reference 28.
[g] Reference 32.
[h] Reference 33.
[i] The quantum defect equals the observed value as the observed ionization energy for the $2s2p\ ^1P$ state is used to adjust the potential employed in this calculation.
[j] Reference 13.

defects against the experimental observed values. The relative accuracy of various theoretical approaches remain at the same level as what we have found for the $2snp\ ^1P$ series. We should note here that a detailed examination of the eigenvectors from our calculation has confirmed the wave-function composition reported by Froese Fischer in her MCHF calculation.[14] In particular, the $2p^2$ contribution to the lowest-energy state in the ^1D series has a value close to 60% which is almost identical to the MCHF result. The quantum defects for the $2s^2\ ^1S$ ground state and a selection of other excited states are listed in Table III. As expected, the overall agreement between the calculated quantum defects and the observed values are improved for those states which are not as

TABLE II. Quantum defects for $2p^2$ and $2snd\ ^1D$ series converging to Be II $2s$ limits. The present (B-spline FCHF) result represents the CI calculations with set of B-spline basis set subject to the ^1S frozen-core Hartree-Fock potential. The present (bound FCHF) result represents the CI calculations with the basis set including only the bound orbits subject to the ^1S frozen-core Hartree-Fock potential.

Theory	$2p^2$	$2s3d$	$2s4d$
Present (B-spline FCHF)	−0.4544	−0.1998	−0.1431
Present (bound FCHF)	−0.4846	−0.2322	−0.1711
Saha and Froese Fischer[a]	−0.4516	−0.2013	−0.1466
Norcross and Seaton[b]	−0.4594	−0.2095	−0.1526
Hibbert[c]	−0.4708		
O'Mahony and Watanabe[d]	−0.475	−0.231	−0.173
Markiewicz *et al.*[e]		−0.0105	−0.0122
Serrao[f]		0.3401	0.4499
Observed[g]	−0.4480	−0.1928	−0.1369

[a] Reference 14.
[b] Reference 12.
[c] Reference 16.
[d] Reference 28.
[e] Reference 33.
[f] Reference 32.
[g] Reference 13.

TABLE III. Quantum defects for selected $^{1,3}S$, ^3P, and ^3D states.

State	Expt.[a]	Present	Ref. 12	Ref. 15	Ref. 16	Ref. 25	Ref. 33
$2s^2\,^1S$	0.7920	0.7912	0.7878	0.7891	0.7898	0.7855	0.7920[b]
$2s3s\,^1S$	0.6873	0.6869	0.6812	0.6827		0.6753	0.6512
$2s4s\,^1S$	0.6787	0.6788	0.6714	0.6626		0.6634	0.6355
$2s5s\,^1S$	0.6765	0.6763	0.6685	0.6546		0.6556	0.6306
$2s3s\,^3S$	0.8210	0.8211	0.8193		0.8168	0.8137	0.8210[b]
$2s4s\,^3S$	0.7955	0.7961	0.7943			0.7826	0.7875
$2s5s\,^3S$	0.7870	0.7879	0.7860			0.7668	0.7772
$2s2p\,^3P$	0.5640	0.5632	0.5625	0.5597	0.5596	0.5502	0.5640[b]
$2s3p\,^3P$	0.4042	0.4036	0.3990	0.3946	0.3936	0.3777	0.4139
$2s4p\,^3P$	0.3815	0.3810	0.3755	0.3678		0.3476	0.3892
$2s3d\,^3D$	0.1101	0.1098	0.1067		0.1011		0.1101[b]
$2s4d\,^3D$	0.1098	0.1092	0.1077				0.1028
$2s5d\,^3D$	0.1099	0.1098	0.1081				0.1006

[a] Reference 13.

[b] The quantum defect equals the observed value as the observed ionization energy of this state is used to adjust the potential employed in the calculation.

strongly correlated as the ^1P and ^1D series.

The $2s^2\,^1S-2s2p\,^1P$ transition in Be is perhaps the most extensively studied transition in alkaline-earth atoms. We have listed the calculated oscillator strengths together with the available excitation energy from a large number of calculations in Table IV. Except from the calculations by Hunter and Berry[30] and by O'Mahony and Greene,[28] the calculated oscillator strengths all agree fairly well with each other and with the experimental measured value.[34] The agreement between most of the calculated excitation energies and the observed value ranges from less than 0.1% to about 3.5% except in the CI calculation by Serrao[32] and the early TDHF calculation by Stewart.[23]

Perhaps the most detailed study among all theoretical calculations for the $2s^2\,^1S-2s2p\,^1P$ transition is the variational Bethe-Goldstone study by Moser *et al.*[18] In particular, by examining the variational results including contribution from the electronic relaxation and correlation at each level of the Bethe-Goldstone hierarchy, Moser *et al.*[18] have concluded that the contribution from the inner-shell effect on the velocity calculation is particularly important in bringing together the length and velocity results. The inner-shell effect in the present calculation is approximated by the localized dipole-polarization potential and the dielectronic interaction discussed in Sec. II. To estimate the contribution of inner-shell effect to the oscillator strengths, we have carried out calculations which exclude these two interactions. The calculated oscillator strengths and the excitation energy *with* and *without* the inner-shell interactions V_p and V_d are listed in Table IV for comparison. Our calculation has shown that the oscillator strengths are reduced by less than 1% when the inner-shell interactions V_p and V_d are included and the disagreement between the length and velocity results is reduced slightly from 4.4% to 4.2%. On the other hand, if one subtracts the inner-shell contributions tabulated by Moser *et al.*[18] from their reported length and velocity oscillator strengths, one gets $f_l=1.41$ and $f_v=1.46$ which are in agreement with our estimation as well as the values reported by Weiss.[15] A similar conclusion has also been made by Hibbert[16] to reduce the calculated oscillator strengths in length and velocity approximations and in bringing f_l and f_v together.

The oscillator strengths for the $2s2p\,^1P-2p^2$ and $2snd\,^1D$ transitions are also strongly affected by the strong mixing between the $2p^2$ and $2snd$ configurations. This group of transitions have been examined in a detailed MCHF calculation by Saha and Froese Fischer.[14] In Table V we have only listed the calculated oscillator strengths from few of the existing calculations. Results from other earlier calculations have been reviewed recently by Saha and Froese Fischer[14] and earlier by Nicolaides and Beck.[20] For the $2s2p\,^1P$ to $2snd\,^1D$ transitions, the results from the present calculation using *B*-spline basis set are in close agreement with the results from the MCHF calculation, and the length and velocity results from the present calculation agree to less than 3%. Our calculated oscillator strength also exhibits the convergence pattern similar to that found in our earlier calculation[2] for Mg as the number of configuration series included in the calculation increases. The calculated average oscillator strengths by Markiewicz *et al.*[33] differ substantially from all other calculated values.

For the weak transition from $2s2p\,^1P$ to $2p^2\,^1D$, the calculated oscillator strengths deviate by orders of magnitude from calculation to calculation. As we increase the number of configuration series, we could not establish the smooth convergence pattern which is the convergence criterion applied to all other transitions in the present calculation. However, our step-by-step calcula-

TABLE IV. The oscillator strengths (f_l for length approximation, f_v for velocity approximation, and f for average of f_l and f_v or oscillator strength from calculations in that f_l equals f_v theoretically) and excitation energy ΔE (in Ry.) for the $2s^2\,{}^1S-2s2p\,{}^1P$ transition for Be I.

Theory	f_l	f_v	f	ΔE
Present (*B*-spline FCHF)	1.3869	1.4496		0.3903
Present (outer correlation only)	1.3986	1.4590		0.3913
Present (bound FCHF)	1.4253	1.3996		0.3943
Moser, Nesbet, and Gupta[a]	1.3862	1.3776		0.3888
Weiss[b]	1.410	1.455		0.3897
Hibbert[c]	1.381	1.435		0.3912
Burke, Hibbert, and Robb[d]	1.4237	1.3862		0.4016
Sims and Whitten[e]	1.344±0.095			0.3882
Vector and Laughlin[f]	1.372			0.3956
Markiewicz *et al.*[g]			1.4697	0.3879[h]
Serrao[i]	1.3494			0.4285
Fawcett[j]			1.356	0.3879[h]
Nicolaides and Beck[k]	1.36	1.46		
Johnson and Huang[l]			1.42	0.402
Stewart[m]	1.378			0.3528
Lin and Johnson[n]			1.38	
Amusia *et al.*[o]			1.36	
O'Mahony and Greene[p]		1.13		
Hunter and Berry[q]	1.15			
Observed[r]			1.34±0.05	0.3879

[a] Reference 18.
[b] Reference 15.
[c] Reference 16.
[d] Reference 34.
[e] Reference 17.
[f] Reference 25.
[g] Reference 33.
[h] ΔE should equal the observed value as the experimental excitation energy of this transition is used to adjust the potential employed in the calculation.
[i] Reference 32.
[j] Reference 27.
[k] Reference 20.
[l] Reference 19.
[m] Reference 23.
[n] Reference 21.
[o] Reference 22.
[p] Reference 28.
[q] Reference 30.
[r] Reference 35.

tion did establish the trend that our length result decreases continuously as we increase the number of configuration series and we could consider the listed length value in Table V the upper bound in the present calculation. Our calculated oscillator strengths are much smaller than the MCHF values but are consistent in order of magnitude with the results from the earlier CI calculations by Hibbert[16] and the variational Bethe-Goldstone calculation by Moser *et al.*[18] The more recent RV result[30] is one to two orders of magnitude larger than all other calculations. We have estimated the numerical accuracy in our oscillator strengths calculation approximately at 10^{-4} and to improve our numerical accuracy would require the use of a substantially smaller radial grid size for our numerical wave function.

The oscillator strengths and the excitation energies for other selected transitions are listed in Tables VI and VII. Again, our calculated oscillator strengths are in good agreement with the more elaborate CI calculations by Weiss[15] and Hibbert.[16] The agreement between our length and velocity results are in general at a level of about 3% or less for all transitions except for some weak transitions with oscillator strengths less than 0.01. Our calculated excitation energies are consistently in better agreement with the experimental values than other calculations listed in Table VI and VII.

The accurate determination of the oscillator strengths is extremely difficult and very few oscillator strengths measurements have been carried out in recent years. Most of the available observed values are derived from

TABLE V. Comparison of the calculated oscillator strengths f for the Be $2s2p\ {}^1P$–$2p^2$ and $2snd\ {}^1D$ transitions. Other earlier theoretical oscillator strengths are reviewed recently in Ref. 14.

Final state		Present	MCHF[a]	FOTOS[b]	RV[c]	Others
$2p^2\ {}^1D$	f_l	0.000 48	0.0016	0.0086	0.064	0.0003[d]
	f_v	0.000 02	0.0010	0.0016		~0
$2s3d\ {}^1D$	f_l	0.4087	0.404	0.64		
	f_v	0.4184	0.425	0.41		
	f_{avg}					0.497[e]
$2s4d\ {}^1D$	f_l	0.1754	0.1808	0.19		
	f_v	0.1804	0.1898	0.16		
	f_{avg}					0.121[e]
$2s5d\ {}^1D$	f_l	0.0836	0.0793	0.08		
	f_v	0.0860	0.0819	0.07		
	f_{avg}					0.05[e]
$2s6d\ {}^1D$	f_l	0.0461	0.0445	0.05		
	f_v	0.0474	0.0454	0.05		
	f_{avg}					0.026[e]

[a] Reference 14.
[b] Reference 20.
[c] Reference 30.
[d] Reference 18.
[e] Reference 33.

TABLE VI. Oscillator strengths f and excitation energy ΔE for selected ${}^1P$–${}^1S$ transitions in Be.

Transition	f_l	f_v	f_{avg}	ΔE(Ry)
$2s2p\ {}^1P$–$2s3s\ {}^1S$				
Present	0.1203	0.1249		0.1072
Weiss[a]	0.127	0.121		0.1061
Victor and Laughlin[b]	0.1485			0.0974
Hunter and Berry[c]	0.0640			
Fawcett[d]			0.141	0.1103
Markiewicz *et al.*[e]			0.14	0.1161
Experiment[f]				0.1104
$2s2p\ {}^1P$–$2s4s\ {}^1S$				
Present	0.0095	0.0106		0.2034
Weiss[a]	0.0091	0.0103		0.2025
Victor and Laughlin[b]	0.0099			0.1926
Fawcett[d]			0.02	0.2077
Markiewicz *et al.*[e]			0.0107	0.2090
Experiment[f]				0.2067
$2s2p\ {}^1P$–$2s5s\ {}^1S$				
Present	0.0034	0.0037		0.2406
Weiss[a]	0.0035	0.0039		0.2393
Victor and Laughlin[b]	0.0041			0.2294
Fawcett[d]			0.009	0.2445
Markiewicz *et al.*[e]			0.003	0.2450
Experiment[f]				0.2438
$2s3p\ {}^1P$–$2s4s\ {}^1S$				
Present	0.2121	0.2177		0.0453
Weiss[a]	0.2230	0.2070		0.0445
Victor and Laughlin[b]	0.2560			0.0416
Markiewicz *et al.*[e]			0.267	0.0366
Experiment[f]				0.0461

[a] Reference 15.
[b] Reference 25.
[c] Reference 30.
[d] Reference 27.
[e] Reference 33.
[f] Reference 13.

TABLE VII. Oscillator strengths f and excitation energy ΔE for selected transitions involving ^3S, ^3P, and ^3D states in Be.

Transition	f_l	f_v	f_{avg}	ΔE (Ry)
$2s2p\ ^3P-2s3s\ ^3S$				
Present	0.0820	0.0845		0.2737
Hibbert[a]	0.0807	0.0836		0.2722
Laughlin *et al.*[b]	0.091			0.2666
Markiewicz *et al.*[c]			0.0787	
Experiment[d]			0.089±0.003	
Experiment[e]			0.075±0.003	
Experiment[f]				0.2743
$2s3s\ ^3S-2s3p\ ^3P$				
Present	1.128	1.141		0.0623
Hibbert[a]	1.198	1.100		0.0624
Laughlin *et al.*[b]	1.138			0.0638
Markiewicz *et al.*[c]			1.159	0.0611
Experiment[f]				0.0622
$2s2p\ ^3P-2s3d\ ^3D$				
Present	0.2938	0.2930		0.3647
Hibbert[a]	0.263	0.256		0.3620
Laughlin *et al.*[b]	0.301			
Markiewicz *et al.*[c]			0.287	
Experiment[d]			0.29±0.01	
Experiment[e]			0.32±0.01	
Experiment[f]				0.3652
$2s3p\ ^3P-2s3d\ ^3D$				
Present	0.5015	0.5007		0.0286
Hibbert[a]	0.528	0.605		0.0278
Laughlin *et al.*[b]	0.524			
Markiewicz *et al.*[c]			0.570	0.0298
Experiment[f]				0.0287

[a] Reference 16.
[b] Reference 25.
[c] Reference 33.
[d] Reference 36.
[e] Reference 37.
[f] Reference 13.

the lifetime measurements using the beam-foil technique.[35-38] As pointed out by Saha and Froese Fischer,[14] the uncertainty of the measured oscillator strengths could increase when the effect due to other decay channels are not included in converting the lifetime data into the oscillator strengths. The results of the present calculation are generally in good agreement with all the available observed oscillator strengths.

The quantitative data presented in this paper have demonstrated the ability of the present theoretical procedure to generate the most accurate energy values and to meet the consistency tests on the oscillator strengths including the agreement between the length and velocity results and the convergence pattern following the criterion we have applied recently.[2] Unlike most of the more elaborate theoretical procedures, the present approach does not require the application of the optimization procedure to the individual states involved in the transition. At an accuracy comparable to or better than many of the most accurate theoretical calculations, the use of a *single* basis set with the same orbital wave functions constructed from B splines has also allowed us to carry out a complete calculation involving a large number of states in a single calculation. In addition, the use of the *quasicomplete* finite basis set has successfully accounted for the *continuum* contribution which was not included in our previous calculation using the *incomplete* bound basis set. A more extensive tabulation of the calculated term values, the excitation energies, and the oscillator strengths involving states of higher n values will be published elsewhere. The extension of the present approach to the theoretical procedure which we have employed successfully in our recent study on the doubly excited autoionization states and the photoionization dominated by these autoionization states is currently in progress.

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