Relativistic configuration-interaction perturbation-theory method with application to intercombination and allowed transitions of light Be-like ions

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We have improved our previous mixed configuration-interaction and perturbation-theory (CI+MBPT) methods by including all second-order Coulomb and lowest-order Breit terms. The method is applied in calculations of $E1$ matrix elements for the two $2s^2 \rightarrow 2s2p$ transitions of light Be-like ions. The results are in good agreement with experiments and other precise calculations. The length and velocity transition amplitudes are also more consistent.

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I. INTRODUCTION

Atomic structure methods for atoms such as helium and alkali metals are well developed and give energies and transition rates that agree precisely with experiment. For other type multielectron atoms, however, theory is less reliable. For example, among *ab initio* theories, a frozen-core configuration-interaction (CI) method, a small-model-space many-body perturbation theory (MBPT) [1,2], multiconfiguration Dirac-Fock (MCDF) for Mg-like ions [3], and multiconfiguration Hartree-Fock (MCHF) for Be-like ions [4] and for neutral calcium [5] are less accurate than one-valence-electron theories. The same can be said about semiempirical calculations discussed by Chen [6] for Be, by Metroy [7] for Ca, and by Dai [8] for Sr. Therefore, the development of precise theory for atoms other than helium or alkali metals, such as divalent atoms, is well motivated.

The development of theory for multivalent atoms is also motivated by fundamental experiments in heavy elements: for example, by parity-nonconservation (PNC) experiments in Tl [9,10], in Bi (discussion is given in Ref. [11]), and in Pb [12]. Heavy open-shell atoms have many common features; however, atoms with three or four electrons outside a core, owing to enormous configuration space and substantial core-excitation effects, are difficult technically. Although *ab initio* calculations for these atoms have been performed, the accuracy is not great and many questions need further investigation. Maybe an exception is Tl (the accuracy of calculations of the weak charge has reached 1% level [13]), which can be considered as both a monovalent and a trivalent atom, and its three-particle valence-valence interaction is not very strong. Because the valence-valence correlations of divalent atoms can be treated completely, studies of these atoms can help to understand various complicated atoms for which PNC and electric-dipole moment (EDM) experiments have been performed or are planned. Another important application of the theory of divalent atoms is to provide transition data needed in cold-collision and Bose-Einstein condensation (BEC) experiments. The prospect for achieving BEC in divalent atoms was discussed in [14,15] and depends (in part) on the size of their van der Waals coefficients. Recent calculations of cold-collision properties of alkaline-earth atoms have been performed by Derevianko *et al.* [16]. There are many other possible direct applications of theories of divalent atoms: for example, by calculating the natural linewidth of $6\,^1S_0 \rightarrow 6\,^1P_0$ transition of Yb atom, Porsev *et al.* [17] proposed ultraprecise Yb atomic clocks.

The construction of theory for open-shell atoms is difficult due to strong valence-core and especially valence-valence interactions. However, the combination of valence-valence CI (vvCI) and MBPT provides unique opportunity to realize advantages of the two powerful methods. Recently, we have developed a computer code based on this principle. We calculated [18] energies and transition rates of neutral Be, Mg, Ca, and Sr and found a good agreement with experiment for allowed transitions; however, the agreement with experiment and gauge invariance was much worse in suppressed transitions. Currently, we would like to investigate possible reasons for the inaccuracy of suppressed transitions and for gauge dependence which could be missing second-order Coulomb and first-order Breit corrections, some asymmetry in truncation, or small denominators in perturbation terms. Because light Be-like ions have very strong suppression and other calculations and accurate measurements exist for them, these ions suit well for the test of our new improved CI+MBPT program. Our method has the advantage that even standard PC computers are suitable for calculations so that it can be adopted by many theorists without special computer resources. Because computation time is only several hours and the CI space is large ($n_{\max}$ can be as large as 25), many transitions and energy levels can be studied if necessary. The precision of intercombination transitions rapidly increases for heavier Be-like ions which have less accurate cancellation of the matrix elements and smaller correlation effects. The code can be applied without change to many other divalent atoms and ions.

The light Be-like ions are relatively well studied theoretically and experimentally. Since these ions have only four electrons, it is possible to predict their properties with multiconfigurational methods such as MCDF [19–22] or MCHF [23]; however, for high precision of intercombination transitions a careful analysis of various correlation and relativistic

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corrections is necessary. Very useful in this respect is a recent high-precision storage-ring measurement by Doerfert *et al.* [24], which gives the rate of the intercombination $2s^2 \rightarrow 2s2p$ transition of berylliumlike carbon, 102.94 ± 0.14 sec^{-1}. This rate is in agreement with the value 102.9 ± 1.5 sec^{-1} obtained by Jönsson and Fischer [22] with the MCDF method, but disagrees by 1.3% with the value obtained by Chen *et al.* [25] in elaborate large-scale (200 000 configurations) relativistic configuration-interaction (RCI) calculations accurate to 0.7%. As pointed out in Ref. [25], despite close agreement with experiment the MCDF method [22] has some unresolved issues: the nonorthogonality of bases, omission of some small effects that could be significant at the 1% level. Other calculations give results with a significant scatter, $70-130$ sec^{-1}. Unfortunately, not all calculations are done systematically for the sequence: for example, it would be interesting to see completely parallel calculations, with the same number of configurations, for B II, where another storage-ring precise measurement exists (Träbert *et al.* [26]), and cancellation effects are stronger making theory more sensitive to small corrections. However, not only do theories have problems; the experiments could be less precise than claimed as well: for example, the ion trap measurement (121 ± 7 sec^{-1} [27]) for carbon is by three standard deviations different from the more precise recent measurement [24].

In addition to testing our theory, we also hope to improve the accuracy of transition rates for Be-like ions which are important for various applications in astrophysics and plasma physics as well as for tests of atomic theories and experiments.

The plan of this paper is the following. First, we will describe briefly our method giving expressions for new corrections. Next, we will consider the allowed $2s^2 \rightarrow 2s2p$ transition in some detail: we will show how to improve the gauge independence of simple vvCI+RPA or more refined CI+MBPT methods, study a convergence pattern, and compare final results with measurements and other calculations. Obviously, if a theory is not able to predict accurately this allowed transition, it will be even more problematic for strongly suppressed transitions. Then we will concentrate on various issues of intercombination transitions. We will test nonrelativistic symmetry of terms, give a breakdown of the contributions of Breit and Coulomb corrections, carefully study the truncation errors, and at the end present our final values and compare them with measurements and several theoretical calculations.

II. COMPUTATIONAL METHOD

A. Previous CI+MBPT program

In our previous paper [18] we included dominant, especially for allowed transitions, contributions such as self-energy, screening, and random-phase approximation (RPA) corrections. We demonstrated good accuracy for energy levels and rates of allowed transitions even in strongly correlated atoms such as Ca and Sr. Briefly, the previous version of our the CI+MBPT method, which we also call the Brueckner-orbital (BO) CI method, consists in constructing a basis out of the Brueckner orbitals, computing the effective Hamiltonian matrix and solving an eigenvalue problem to obtain coupled two-valence-electron wave functions. The effective Hamiltonian contains the first-order Coulomb and the second-order screening corrections. RPA corrections are included at the stage of calculations of transition amplitudes.

Despite good agreement with experiment for allowed transitions, we observed some discrepancy for suppressed transitions. Especially large disagreement was in the case of the $2s^2 \rightarrow 2s2p$ intercombination transition of Be-like carbon [28], which is known accurately. Reasons for this discrepancy could be at least four: (1) missing Breit and/or some second-order Coulomb corrections, (2) truncation errors which can result in asymmetry of $l+1/2$ and $l-1/2$ contributions, (3) small denominators that can also amplify the asymmetry between $l+1/2$ and $l-1/2$ states, and (4) incompleteness of the basis. Therefore, we would like to investigate these questions and to improve our previous CI+MBPT code.

B. Inclusion of Breit and second-order Coulomb corrections

The importance of relativistic corrections such as spin-other-orbit and spin-spin terms that come from the Breit operator for the intercombination line in Be-like systems was pointed out by [29]. In a recent paper Chen *et al.* [25] have shown that the Breit contribution to the transition rate of C III is approximately 26% in the four-electron Durac-Kohn-Sham or the three-electron modified-core Hartree potential. Although we use the two-electron Dirac-Hartree-Fock (DHF) potential, we expect that the Breit correction in our case is at the same level and must be included. The missing Coulomb second-order corrections are expected at a few percent level, which also can be inferred from Ref. [25].

We complete second-order contributions to the energy in the CI+MBPT formalism by adding one Coulomb term (with double-core summation). The formula for this term can be found in Ref. [2]:

$$V^{(2)}_{v'w'vw} = \eta_{v'w'}\eta_{vw}\sum_{kbc}(-1)^{j_v+j_c+k+J}\begin{Bmatrix} j_v & j_w & J \\ j_c & j_b & k \end{Bmatrix} \times \frac{X_k(bcvw)Y_J(v'w'bc)}{\varepsilon_b+\varepsilon_c-\varepsilon_{w'}-\varepsilon_{v'}}. \quad (1)$$

The notations are similar to those in the paper. The summation runs over core states b and c as well as over the angular momentum k. The initial v, w and final v', w' states which belong to the model valence-valence CI space have been coupled to the angular momentum J. The normalization coefficient η_{vw} is equal $1/\sqrt{2}$ for two identical states and 1 for not identical.

We include all first-order Breit corrections, which are two. The formula for the first Breit correction,

$$V^{B1}_{v'w'vw} = \eta_{v'w'}\eta_{vw}\sum_{k}(-1)^{j_{w'}+j_v+k} \times \left[(-1)^J\begin{Bmatrix} j_{v'} & j_{w'} & J \\ j_w & j_v & k \end{Bmatrix}B_K(v'w'vw) + \begin{Bmatrix} j_{v'} & j_{w'} & J \\ j_v & j_w & k \end{Bmatrix}B_K(v'w'wv)\right], \quad (2)$$

is obtained from the formula for the first-order Coulomb correction in the DHF V^{N-2} potential by replacing usual Coulomb matrix elements $X_K(ijkl)$ with the Breit matrix elements $B_K(ijkl)$ which consist of three magnetic Slater integrals $M_L(ijkl)$, $N_L(ijkl)$, and $O_L(ijkl)$ defined in Johnson *et al.* [30]:

$$X_L(ijkl) \rightarrow B_L(ijkl) = M_L(ijkl) + N_L(ijkl) + O_L(ijkl). \quad (3)$$

The second Breit correction, which is natural to call Breit-Dirac-Hartree-Fock (BDHF) correction, is defined as

$$B_{ij}^{DHF} = \delta_{j_i j_j} \sum_a \sqrt{\frac{[j_a]}{[j_i]}} \widetilde{B}_0(iaja), \quad (4)$$

where the function $\widetilde{B}_J(ijkl)$ is similar to the function $Z_J(ijkl)$ except that the Coulomb interaction is replaced with the Breit interaction. This correction can be incorporated in all orders automatically if we replace the DHF basis with the BDHF basis. We constructed this basis by diagonalizing the single-particle Hamiltonian

$$h_{ij} = \epsilon_i \delta_{ij} + B_{ij}^{DHF}. \quad (5)$$

Since our basis does not contain negative-energy (NE) states, it will be slightly different than the basis formed by solving the DHF differential equation which contains the Breit interaction. Another way to incorporate BDHF correction is by adding the term

$$V_{v'w'vw}^{BDHF} = \eta_{v'w'}\eta_{vw}[\delta_{w'w}B_{v'v}^{DHF} + \delta_{v'v}B_{w'w}^{DHF} + (-1)^J(\delta_{w'v}B_{v'w}^{DHF} - \delta_{v'w}B_{vw'}^{DHF})] \quad (6)$$

to the two-particle effective Hamiltonian. In this case the higher-order terms that have the summation over intermediate core states will not be included. Since the BDHF correction to nonrelativistically forbidden $E1$ transitions is relatively large, it is important to include it in all orders. For example in C III, the matrix element calculated in the BDHF basis is by several percent smaller than that obtained using Eq. (6) at the level of vvCI, but the results agree well after adding all other corrections because self-energy and screening corrections are also significantly reduced.

We also calculated the Breit RPA correction (in the RPA diagram a Coulomb line is replaced with a Breit line)

$$\langle w\|z^{BRPA}\|v\rangle = \sum_{an} (-1)^{a-n+J} \frac{1}{[J]} \left[\frac{\langle a\|z^{RPA}\|n\rangle \widetilde{B}_J(wnva)}{\epsilon_a - \epsilon_n - \omega} + \frac{\widetilde{B}_J(wavn)\langle n\|z^{RPA}\|a\rangle}{\epsilon_a - \epsilon_n + \omega} \right], \quad (7)$$

which turned out to be important only for the velocity form. Including this correction without including NE contributions introduces strong disagreement between length and velocity forms for the intercombination transitions. Our result for C III has the difference between length and velocity forms close to that observed in Ref. [25] before the NE correction was added. The difference would decrease substantially if we added second-order NE contributions. However, even with NE contributions added in Ref. [25] the agreement was only about 6% in three-electron modified core Dirac-Hartree (MCH) potential calculations which might indicate that higher-order NE effects are important. How to add NE corrections beyond the second order is an open question which requires additional work, but if only second-order NE corrections are used, velocity form results can be inaccurate. By this reason we will present only length-form results for comparison with other calculations and with experiment.

We also find that it is important to use retarded matrix elements (equations for reduced matrix elements with retardation can be found in [31]) in calculations of nonrelativistically forbidden transitions: the retardation contribution to the rate of the C III intercombination transition is 2%. The allowed transitions are insensitive to the retardation, at least for the low-Z ions considered here.

III. CALCULATIONS FOR THE ALLOWED TRANSITION

A. Completeness of the spline basis and cavity effects

Although light Be-like ions have the convergence pattern for matrix elements of the allowed transition and for energies of lowest states quite similar, the B II and C III ions require more careful consideration to account for larger correlation effects. Once the convergence is achieved for these ions, the number of configurations and other parameters of calculations can be kept the same, except that the cavity sizes should be rescaled. The dipole matrix elements of the allowed transition and the transition energies of $^3P_1$ and P_1 states do not change significantly when we vary the maximum principal quantum number of spline orbitals, n, included CI+MBPT from 13 to 18 and the cavity size R_{cav} in which splines are generated from $24/Z^{ion}$ to $45/Z^{ion}$ a.u. After an additional analysis (it is given in a separate section) of the convergence of intercombination transitions, which are more sensitive to completeness of the basis, we find that $R(Z^{ion}) = 24/Z^{ion}$ and $n_{max} = 18$ are optimal for the resonance and intercombination transitions for all ions; these parameters will be used in final calculations.

B. Length form vs velocity form

In the literature electric-multipole matrix elements are very often calculated in the length form (in MCDF the Babushkin gauge) and the velocity form (in the MCDF the Coulomb gauge), and the accuracy of calculations is often estimated from the length-velocity difference, so it is important to understand which form, length or velocity, is more accurate and what does the difference mean. Because the velocity matrix element V_{ij} is proportional to the energy difference $\epsilon_i - \epsilon_j$, many diagrams that involve states with large energies are more significant in velocity form, making it more "dangerous" when not all terms are collected order by order. Furthermore, the length-velocity disagreement does not give the accuracy of calculations, but merely the inaccuracy of the velocity form. This fact is obvious because form-independent order-by-order MBPT can be constructed [32,33]. In a CI+MBPT method some diagrams are omitted while others are treated in all orders; therefore, we expect that the velocity form can be problematic. In other methods

the situation is often similar, the length-form result is more accurate than the velocity, but the analysis is required. For example, if we consider convergence with increasing number of configurations in the CI method, highly excited states in the cavity have large energies and will be more important for the velocity form. This is also true for the contributions from the negative-energy continuum. When nonlocal potentials and/or all-order methods are used, it might be difficult to choose more accurate form or to achieve form independence. However, it is desirable to have complete agreement between gauges to check code errors and the completeness of the basis or to use the program to calculate magnetic transitions which do not have length form matrix elements.

Can CI+MBPT formalism be made form independent with high accuracy? We do not have an answer to this important question yet, but we have a good starting point. If RPA corrections are included in valence-valence CI calculations, disagreement of the order of a few percent is observed, but adding the diagram below makes agreement of forms at the level better than 0.1%:

$$Z^{corr,a}_{v'w'vw} = \sum_{ka} (-1)^{1+k+J+j_w+j_{w'}} \frac{Z^{RPA}_{av} X_k(v'w'wa)}{\epsilon_a+\epsilon_w-\epsilon_{v'}-\epsilon_{w'}} \times \begin{Bmatrix} J & J' & 1 \\ j_a & j_v & j_w \end{Bmatrix} \begin{Bmatrix} j_a & j_w & J' \\ j_{v'} & j_{w'} & k \end{Bmatrix} + \sum_{ka} (-1)^{1+k+j_v+j_{v'}} \frac{Z^{RPA}_{v'a} X_k(aw'vw)}{\epsilon_a+\epsilon_{w'}-\epsilon_v-\epsilon_w} \times \begin{Bmatrix} J' & J & 1 \\ j_a & j_{v'} & j_{w'} \end{Bmatrix} \begin{Bmatrix} j_a & j_{w'} & J \\ j_w & j_v & k \end{Bmatrix}, \tag{8}$$

$$Z^{corr,a}_{JJ'} = \sqrt{(2J+1)(2J'+1)} \sum_{vwv'w'} \eta_{vw}\eta_{v'w'} C^J_{vw} C^{J'}_{v'w'} \times [Z^{corr,a}_{v'w'vw} + (-1)^{j_{v'}+j_{w'}+J'+1} Z^{corr,a}_{w'v'vw} + (-1)^{j_v+j_w+J+1} Z^{corr,a}_{v'w'wv} + (-1)^{j_{v'}+j_{w'}+j_v+j_w+J+J'} Z^{corr,a}_{w'v'wv}]. \tag{9}$$

Here C^J_{vw} and $C^{J'}_{v'w'}$ are configuration weights of the initial and final states coupled to the total angular momenta J and J', respectively. Roughly speaking, this term is what is left (NE contributions are not important for allowed transitions) in the second order from the term Z^{corr} given in Ref. [34] if we use valence-valence CI wave functions in calculations of matrix elements—that is, in the initial summation over all indices i the summation over excited states is automatically included in CI, but the summation over core and NE states is not. This term is small in the length form and can be neglected. However, it is important for the velocity-form amplitude. Why does this correction improve significantly the gauge invariance of the valence-valence CI+RPA? To understand this we have to look at a simpler two-electron atom. It was demonstrated numerically and proved analytically by Johnson *et al.* [31] that two-electron CI matrix elements are accurately form independent if negative-energy corrections are added. To prove form independence (FI) the following commutator of the interaction potential with the gauge operator Ξ was introduced:

$$[V,\Xi] = \frac{1}{2}\sum_{ijkl} O_{ijkl} a_i^\dagger a_j^\dagger a_l a_k, \tag{10}$$

where

$$O_{ijkl} = \sum_r \{v_{ijrl}\zeta_{rk} + v_{ijkr}\zeta_{rl} - \zeta_{ir}v_{rjkl} - \zeta_{jr}v_{irkl}\}. \tag{11}$$

This commutator will vanish if the index r runs over all positive and negative states. In two-electron CI the basis is formed from positive-energy states and the commutator does not vanish. In order to complete the summation over NE states, the second-order NE contribution was added perturbatively and form independence was improved even in intercombination transitions. In the valence-valence CI, the summation over intermediate NE and core states is also missing. Therefore, we added the second-order diagram, Eq. (9), to restore the summation over a complete positive spectrum. Unlike the case of helium, we use nonlocal DHF potential, and in order to have FI of one-particle matrix elements necessary for the proof of FI of the two-particle matrix elements, instead of "bare" we have to use "dressed," full RPA matrix elements which satisfy the relation

$$V^{RPA}_{ij} = \omega_{ij} Z^{RPA}_{ij}. \tag{12}$$

The full RPA correction can be obtained by iterating core RPA until the convergence is reached. In the case of allowed transitions, NE contributions scale as $\alpha^2 Z$, so even not including NE contribution it should be possible to achieve the relative form difference at the level 10^{-4}. Typical differences between length and velocity matrix elements are shown in Table I. Because the completeness of the basis is important, we vary l_{max}, n_{max} of RPA matrix elements that replace first-order matrix elements, the number of core RPA iterations, and n_{max} of the term defined by Eq. (9). It is somewhat strange that when the basis is the most complete, we obtain the L-V agreement only at the level of 0.1%, while by restricting the basis we achieved 10 times better agreement. One reason for the residual disagreement can be the uncertainty in the denominators of MBPT corrections. To avoid

TABLE I. The form independence of the matrix elements for the B II resonance transition. N_{RPA} is $n_{\max}$ of RPA matrix elements that replace first-order matrix elements, $N_{coreRPA}$ is the number of iteration of core RPA, and N_{Zcore} is the maximum n of the term defined in Eq. (9).

$l_{\max}$	N_{RPA}	$N_{coreRPA}$	N_{Zcore}	$L-V$
3	10	10	10	0.00015
3	15	30	15	0.00076
4	10	10	10	0.0016
4	15	30	15	0.002
5	10	10	10	0.0015
5	15	30	15	0.0024

closeness to zero we replace each denominator in Eq. (9) with the denominator in which the initial valence state is the lowest excited state for a given j. Thus the denominator is always negative. Still not including corrections from Eq. (9) would make disagreement at the level of 1%. A similar situation for the allowed transition of C III and other ions (see Table II). In this table we also show the length-velocity agreement for intercombination transitions, which is surprisingly good starting from O V, considering the fact that we omitted NE corrections. Without NE contributions, as we already discussed, the BRPA correction becomes problematic leading to large L-V disagreement, so that to achieve better gauge invariance, we decided to exclude BRPA correction. The contribution from Eq. (9) is small to intercombination transitions in the length form and can be neglected. The velocity form correction is substantial, but does not improve form independence for low-Z ions.

C. Comparison for oscillator strengths

Since there are many calculations and experiments available, it is interesting to compare our results with the results of others. In Table III, we give a comparison for oscillator strengths of the allowed $2s^2 \rightarrow 2s2p$ transition. The accuracy of our CI+MBPT calculations is expected at the level 0.1%. We agree with elaborate RCI calculations by Chen *et al.* [25] within our estimated error and with most calculations given in the table at the level 0.2% as well as with experiment within experimental error bars. For example, we have good agreement with recent, refined MCDF calculations by Jönsson *et al.* [19] for four ions, including Fe XXIII. The comparison for this ion is of interest to check relativistic corrections. In O V, the MCDF method of Ref. [20] gives result different from ours by 0.65%, while we agree well with other calculations for this ion. More calculations for this allowed transition can be found following Ref. [19].

IV. CALCULATIONS FOR THE INTERCOMBINATION TRANSITION

A. Nonrelativistic limit test

Because any small asymmetry of contributions from $l+1/2$ and $l-1/2$ states can result in a large error for intercombination transitions which have strong cancellations, we designed a simple test to check for the asymmetry. We replaced radial wave functions and energies of $l+1/2$ states with those of $l-1/2$ states at different stages of calculations. Thus after this nonrelativistic symmetrization, matrix elements calculated with the frozen-core valence-valence CI became very small, less than 10^{-6} a.u. We tested each diagram and found that the screening correction gave anomalously large value, up to 10^{-4} a.u. Because the truncation was completely symmetric, by fixed orbital angular momentum of relativistic states, it was difficult to explain this effect. It turned out that the problem was in the denominators. When highly excited states are included into the effective Hamiltonian, the denominator of the screening correction $\varepsilon_\alpha+\varepsilon_b-\varepsilon_{\beta'}-\varepsilon_n$, where α and β' belong to excited states included into vvCI, can become small accidentally. When we used instead of this denominator the denominator $\varepsilon_b-\varepsilon_n$, the

TABLE II. The form independence of the allowed (L_A, V_A) and intercombination (L_F, V_F) matrix elements for Be-like ions. The parameters of the calculations are standard: $n_{\max}=18$, $l_{\max}=5$, optimized cavity sizes; all corrections considered in this paper except for BRPA are included; N_{Zcore}, $N_{coreRPA}$, and N_{RPA} defined in Table I are equal 10. Small in length form but large in velocity form BRPA correction is not included because it completely destroys form invariance of the intercombination transitions for low-Z ions due to its large NE contribution. The ratio of matrix elements of the allowed to the intercombination transition shows the degree of suppression of the intercombination transition which is somewhat correlated with form independence and which is important for understanding the accuracy of the intercombination transitions. Numbers in square brackets denote powers of 10.

Ion	L_A	L_A-V_A/L_A	L_F	L_F-V_F/L_F	L_A/L_F
B II	2.1177	−0.0015	4.99[−4]	0.150	4244
C III	1.5618	−0.0020	9.94[−4]	0.061	1571
N IV	1.2402	−0.0022	1.64[−3]	0.052	757
O V	1.0299	−0.0023	2.43[−3]	0.001	423
F VI	0.8813	−0.0023	3.37[−3]	−0.001	261
Ne VII	0.7707	−0.0023	4.46[−3]	−0.002	173
Fe XXIII	0.2594	0.0000	3.71[−2]	0.002	7

TABLE III. Comparison of oscillator strengths for the allowed $2s^2 \rightarrow 2s2p$ transition of Be-like ions. Theoretical results are given in the length or equivalent Babushkin gauges, the velocity and equivalent Coulomb gauge results are disregarded.

	CI+MBPT	MCDF[a]	MCDF	CIV3	RCI[b]	Experiment
B II	0.9998		1.0012[c]	0.994[d]		0.971±0.079[e]
C III	0.7583		0.7571[f]	0.757[g]	0.7577	0.753±0.026[h]
N IV	0.6106	0.6117	0.6099[f]	0.609[i]		0.620±0.022[j]
O V	0.5116	0.5123	0.5081[f]	0.511[d]		0.528±0.023[j]
F VI	0.4408					
Ne VII	0.3878	0.3882		0.387[d]		0.420±0.067[k]
Fe XXIII	0.1538	0.1539				0.156±0.015[l]

[a]Jönsson *et al.* [19].
[b]Chen *et al.* [25].
[c]Ynnerman and Fischer [21].
[d]Fleming *et al.* [35].
[e]Bashkin *et al.* [36].
[f]Ynnerman and Fischer [20].
[g]Fleming *et al.* [37].
[h]Reisted *et al.* [38].
[i]Fleming *et al.* [39].
[j]Engström *et al.* [40].
[k]Irwin *et al.* [41].
[l]Buchet *et al.* [42].

problem was instantly solved: the nonrelativistic substitution made the screening correction very small. However, according to the rules of MBPT, such a denominator is wrong. The compromise solution, which would be almost correct for the ground and lowest excited states, is to replace α with the lowest excited states of given j_α. Thus denominators will be always negative, and its value will be correct for dominant contributions. The nonrelativistic asymmetry from the corrected denominators becomes small, and we used the screening term with these denominators in all subsequent calculations.

B. Truncation errors for the intercombination transition

Forbidden transitions are very sensitive to various truncation errors. Because of memory restrictions of our particular computer, it was necessary to keep the number of valence-valence configurations less than 5000. We restricted $l_{\max}$ to 5 and $n_{\max}$ to 18. By reducing the cavity size we made this basis complete enough to account for correlations of lowest excited states. Table IV illustrates variations of results with $l_{\max}$, $n_{\max}$, and R_{cav}. First of all, we can see that $n_{\max}=18$ and the cavities 15 a.u. for B II and 10 a.u. for C III are almost optimal since further reduction of the cavity from 15 to 14 for B II and from 10 to 8 for C III does not change result. In addition, decrease of $n_{\max}$ from 18 to 17 ($R_{cav}=14/8$ for B II/C III) changes the result only by 1×10^{-6}. Because energies of an ion in a cavity starting from some n grow very rapidly, the correlation corrections are suppressed by large denominators and decrease rapidly, too.

It also can be concluded that $l_{\max}=5$ is sufficient if we add the value from extrapolation to infinite $l_{\max}$ equal about 1×10^{-6} for B II and 3×10^{-6} for C III. For transition rates these corrections will be 0.4% and 0.6%, respectively. A similar correction from l extrapolation for C III, 0.56%, was estimated in Ref. [25]. We have some concern about the B II l-extrapolation correction, which might be larger, since we found that for appropriate extrapolation $n_{\max}$ should be sufficiently large; $n_{\max}=18$ barely satisfies the completeness condition for $l_{\max}=5$. The extrapolation problem can be seen

TABLE IV. Cavity and truncation effects. The effective Hamiltonian matrix is truncated by the maximum angular momentum $l_{\max}$ and by the maximum number of excited states $n_{\max}$ for a given $j=l\pm1/2$: the total number of relativistic single-particle states is $(2l_{\max}+1)n_{\max}$ and the number of two-particle states is less than 5000. The retarded reduced matrix elements in the length form (RME) and the cavity radii R_{cav} are given in atomic units; $n_{\max}$ and $l_{\max}$ are the same for B II and C III on each line, while the cavity sizes are different

$n_{\max}$	$l_{\max}$	R_{cav}	RME	R_{cav}	RME
			B II		C III
18	2	15	0.000500	10	0.000989
18	3	15	0.000509	10	0.001005
18	4	15	0.000511	10	0.001010
18	5	15	0.000512	10	0.001012
17	5	15	0.000510	10	0.001011
18	5	14	0.000512	8	0.001012
17	5	14	0.000511	8	0.001011

TABLE V. Breakdown of contributions to the reduced matrix element for B II and C III: vvCI, BDHF, and RPA are treated in all orders; the most important are two-particle Breit (Br 2), Brueckner-orbital (BO), the screening (Scr), and the matrix-element retardation (RME) corrections. All values should be multiplied by 10^{-6} a.u.

Corrections	Value	B II Total	Value	C II Total
vvCI+BDHF+RPA		448		906
+BO	23	471	26	932
+Scr	−13	458	8	940
+CC	0	458	1	941
+Br 2	41	499	53	994
+RME	9	508	10	1004
+BRPA	−1	507	−1	1003
+Extrap $l>5, n>18$	1+3	510	3+3	1009

from the decrease of energies of the states with l for a fixed $n=18$: for $l=2,3,4,5$ we obtain approximately energies 119, 152, 28, 33 a.u. Extrapolation to infinite n can be warranted, but the dependence on n is not as smooth as on l so that we give only approximate estimates: for B II and C III the increase of the matrix element is about 3×10^{-6} a.u. For heavier ions relative importance of the truncation errors decreases rapidly with Z for the chosen optimal basis as the transition becomes less suppressed (see Table II where the ratios of the allowed to the intercombination transitions are given).

C. Breakdown of contributions to the intercombination transition

To understand the most important corrections and the accuracy of our calculations in Table V we show the breakdown of contributions of the MBPT terms. The BDHF correction is dominant correction beyond Coulomb vvCI approximation, and it was included in all orders by using the BDHF basis. The second Breit correction, in the table denoted as "Br 2" and defined by Eq. (2) is also very important. Among second-order Coulomb correlation corrections, as usual, Brueckner orbital and screening, are dominant. Note that the screening correction changes sign from C III to B II which is due to partial cancellation of low-n and high-n contributions. The extrapolation to infinite $l_{\max}$ and $n_{\max}$ is also significant.

D. Length-velocity agreement

Length-velocity agreement for allowed and intercombination matrix elements has been shown in Table II. It is not surprising that in general the agreement for allowed transitions is much better since the intercombination transitions are very sensitive to various relativistic and correlation corrections, in particular to NE contributions. The largest deviation of results is obtained for the B II intercombination transition, 15%, but for O V–FE XXIII ions, the length and velocity form results agrees at 0.2% level. Such an agreement for the intercombination transitions is rather unexpected. It is interesting to note that the addition of BRPA correction does not improve agreement but instead makes it much worse. For example, with this diagram included the C III rate calculated from the velocity matrix element is approximately 190 $\sec^{-1}$, much different from 100 $\sec^{-1}$ in the length form, but close to the result obtained by Chen *et al.* [25] in velocity form before NE corrections were added. Since major part of disagreement arrives with BRPA correction, one can conclude that the dominant NE contribution must be contained in this diagram. It would be interesting to verify this conclusion.

The BRPA diagram is small in the length form and it does not matter if we include or ignore it in our calculations. In fact, we believe that the velocity form result will be more accurate if we omit this correction. This conclusion might be useful for calculations of magnetic-multipole transitions for which the length form does not exist. Note that NE contributions would be automatically included if we solved the differential RPA equations; then the complete RPA correction, including BRPA, becomes form independent, and will be safe for the velocity form. Because in the MCDF method, some corrections are included by solving differential equations corresponding to these corrections NE contributions are also included automatically, and approximate gauge invariance can be achieved. However, correction based on a diagonalization of the Hamiltonian matrix built on the basis of positive-energy states are not necessary gauge independent. Because the velocity form is always more sensitive to NE corrections, the accuracy of the results cannot be judged by looking at length-velocity difference or having good form independence does not always mean good accuracy, especially for intercombination transitions.

E. Comparison for the rates of the intercombination transition

Transition rates of intercombination transitions are compared in Table VI. In the case of C III, we find a 1%–5% deviation from other calculations and experiments, which is the level of disagreement of other precise calculations presented in the table. For B II, which has the strongest cancellation, our theory is off from experiment by 8% which is the accuracy of our calculations estimated from the analysis of MBPT corrections, $l_{\max}$ and $n_{\max}$ interpolation, and isoelectronic comparison. It would be interesting to see the results of calculations performed with large-scale RCI method of Ref. [25] which carefully takes into account relativistic and correlation effects. For N IV and O V, we agree well with MCDF calculations by Jönsson and Fischer [22] and Doerfert *et al.* [43] and not very accurate experiments. We also agree well, the within 0.7%, with the MCDF of Jönsson and Fischer [22] for Fe XXIII. On the other hand, the CIV3 method does not agree as precisely with our calculations and MCDF for N IV and O V.

The C III intercombination transition has been studied in more than 16 theoretical works. The early calculation with CI method published in 1972 gave 77 $\sec^{-1}$, other results are distributed in the range 77–118 $\sec^{-1}$. This large dispersion occurs due to very high sensitivity of the C III intercombi-

TABLE VI. Comparison of transition rates for the intercombination $2s^2 \rightarrow 2s2p$ transition of Be-like ions. Theoretical results are given in the length or equivalent Babushkin gauges; the velocity and equivalent Coulomb gauge results are disregarded. The experimental energy is used to calculate rates from CI+MBPT line strengths. The error of our CI+MBPT result for C III is estimated from the truncations error, about 0.5%, from the value of the omitted diagrams, about 1%, and from comparison with precise theory [25] and experiment [24]. For other ions relative errors where scaled by the degree of cancellation of matrix elements. Brackets denote powers of 10.

	CI+MBPT	MCDF[a]	MCDF	MCDF[b]	CIV3	RCI[c]	Experiment
B II	9.2±0.7		9.99[d]		9.73[e]		10.24±0.05[f]
C III	99±3		100.3[g]	102.9	104.4[h]	101.6±0.7	102.94±0.14[i]
N IV	565±8	558.6	556.3[g]		577.0[j]		625±150[k]
O V	2229±18	2212	2207[g]		2280[e]		2000±400[k]
F VI	7022±35	6961					
Ne VII	1.89±0.06[4]	1.862[4]			1.92[4][e]		2.2±1.1[4][l]
Fe XXIII	5.22[7]			5.186[7]			5.71±0.5[7][m]

[a]Jönsson *et al.* [19].
[b]Jönsson and Fischer [22].
[c]Chen *et al.* [25].
[d]Ynnerman and Fischer [21].
[e]Fleming *et al.* [35].
[f]Träbert *et al.* [26].
[g]Ynnerman and Fischer [20].
[h]Fleming *et al.* [37].
[i]Doerfert *et al.* [24].
[j]Fleming *et al.* [39].
[k]Doerfert *et al.* [43].
[l]Kunze [44].
[m]Hutton *et al.* [45].

nation transition to various correlation and relativistic corrections. For example, we already mentioned the importance of Breit interaction, so calculations that do not include this interaction are not accurate. In addition, valence-core interaction plays an important role as well. So in order to judge the accuracy of methods, it is important to see the breakdown of various effects and the convergence with an increase of the basis. In MCDF methods, there exists also a problem of nonorthogonality of separately optimized states. Because in our calculations we included all most important contributions and studied truncation errors, we believe that our results and error estimates are reliable. Relatively large errors for B II can be explained by strong cancellations which make the result sensitive to small asymmetry in the treatment of relativistic states of type $j=l+1/2$ and $l-1/2$, which we tried to avoid by truncating states with condition $l<l_{\max}$ and to correlation and relativistic effects. Although it is not possible to include all MBPT and relativistic corrections, we made estimates of omitted diagrams. For example, the Breit corrections to important second-order self-energy and screening diagrams are at the level less than 0.5% for B II and C III, and even smaller is the contribution from the third-order structure-radiation correction. So the overall error from the omitted diagrams is expected at the level of 1% for B II and C III. For heavier ions, our calculations improves precision rapidly as the cancellation of matrix elements decreases and agree well with other elaborate calculations. Our current theory can be improved in several ways. One interesting approach would be to test various starting potentials, which are better than two-particle DHF and would lead to faster convergence of CI. The positive effects from optimized potentials should be most important for B II. Another improvement possible from optimizing denominators in the screening correction. Some higher-order diagrams can be also necessary to consider.

V. CONCLUSION

In this paper, we presented relativistic CI+MBPT transition probabilities (oscillator strengths) for the $2s$-$2p$ transitions of berylliumlike ions. We find our results in close agreement with experiments and other elaborate theories although the B II intercombination transition has relatively large uncertainty. To improve accuracy and form independence, we modified our previous code to include all second-order Coulomb and dominant Breit corrections. The equations for these corrections and their values are provided. One important conclusion from this work is that CI+MBPT method can be used in calculations of suppressed transitions which are very often of interest for many applications.

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