

Energy levels and transition amplitudes for alkali-metal atoms in the Brueckner approximation

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We use the B -spline approximation to solve the Brueckner equation. The Brueckner equation is obtained from Dyson equation for the one-particle propagator by cutting the kernel at second order in the electron-electron interaction. Thus the Brueckner approximation is a straightforward extension of the frozen-core Dirac-Fock approximation to include second-order correlations in a self-consistent way. We also give the explicit expression for the gauge-invariant transition in the Brueckner approximation. The numerical results of energies and transition amplitudes for alkali-metal atoms in the Brueckner approximation differ from experimental values by percentages ranging from 0.1% to 2%, increasing from Li to Cs. These results are comparable to existing accurate theoretical values.

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I. INTRODUCTION

For the alkali-metal atoms, the simplest nontrivial approximation is the (frozen-core) Dirac-Fock (DF) approximation in the relativistic case. This approximation is historically derived from the variational method to yield a differential equation for one-particle orbitals, namely, the DF equation. The DF equation can be solved numerically without difficulty. Energy levels and transition amplitudes in the DF approximation differ from experimental values by 1–10% for the alkali-metal atoms [1].

One way to improve theoretical values for energy levels and transition amplitudes is using the many-body perturbation theory (MBPT) to compute the high-order contributions [2]. Blundell, Johnson, and Sapirstein have shown that the energy levels can be brought to within 1% error of experimental values for some valence states of alkali-metal atoms if up to third-order corrections in MBPT are included [3]. However, the perturbative corrections to the transition amplitudes are known not to produce results as good as in the case for energy levels. Explicit perturbative calculations up to second order, using the DF orbitals, for some transition amplitudes of Cs were given in our previous work [4]. In that work one clearly saw that infinite subsets of high-order contributions have to be included in order to get good results for transition amplitudes. As we have mentioned in previous work [4], one of such infinite subsets of high-order contributions comes from random-phase-approximation-(RPA)-type contributions [5]. Another comes from using the Brueckner orbitals [6]. The RPA-type contributions for alkali-metal atoms have been given in Ref. [7]. In this paper we use the Brueckner orbitals to compute transition amplitudes for alkali-metal atoms. In Sec. II we define the Brueckner approximation using a Green's-

function formalism [8]. Numerical results with a discussion are presented in Sec. III. We conclude our work in Sec. IV.

II. THE BRUECKNER APPROXIMATION

A. Energies and wave functions

From the field-theoretical approach, the one-particle orbitals can be obtained by considering a one-particle propagator [8]. The exact one-particle propagator satisfies Dyson's equation,

$$G_1 = G_1^{(0)} + G_1^{(0)} K G_1, \quad (1)$$

where $G_1^{(0)}$ is the one-particle propagator with the electron-electron interaction V neglected. The kernel in Dyson's equation can be expanded order by order in V :

$$K = \Sigma^{(1)} + \Sigma^{(2)} + O(V^3). \quad (2)$$

Dyson's equation can be solved approximately by cutting the kernel K at some order of V . Accordingly, we will call the approximation n th order if $(n+1)$ th and higher-order terms in kernel K are neglected. The zeroth-order approximation is clearly the independent-particle approximation. Its corresponding one-particle orbitals are hydrogenic. The first-order approximation has been shown to yield the DF equation [8]. Using the same technique employed in Ref. [8], one can easily show that under second-order approximation the wave functions satisfy the following equation:

$$(\epsilon_v - H_0)|v\rangle = \Sigma^{(1)}|v\rangle + \Sigma^{(2)}|v\rangle, \quad (3)$$

where H_0 is hydrogenic Hamiltonian. ϵ_v is the term energy of orbital $|v\rangle$. $\Sigma^{(1)}|v\rangle$ and $\Sigma^{(2)}|v\rangle$ are given by

$$\Sigma^{(1)}|v\rangle = \sum_a [\langle a \cdot | V | a v \rangle], \quad (4)$$

$$\Sigma^{(2)}|v\rangle = \sum_{a,i,j} \frac{\frac{1}{2}}{\epsilon_v + \epsilon_a - \epsilon_i - \epsilon_j} [\langle a \cdot | V | ij \rangle][\langle ij | V | a v \rangle] + \sum_{a,b,i} \frac{\frac{1}{2}}{\epsilon_v + \epsilon_i - \epsilon_a - \epsilon_b} [\langle i \cdot | V | ab \rangle][\langle ab | V | i v \rangle], \quad (5)$$

with $\langle m \cdot |V|st \rangle$ and $\langle mn|V|st \rangle$ defined as

$$\langle m \cdot |V|st \rangle = \left[\int \Psi_m^\dagger(\mathbf{r}')V(\mathbf{r}-\mathbf{r}')\Psi_s(\mathbf{r}')d\mathbf{r}' \right] \Psi_t(\mathbf{r}) \quad (6)$$

and

$$\langle mn|V|st \rangle = \int \Psi_m^\dagger(\mathbf{r}')\psi_n^\dagger(\mathbf{r}'')V(\mathbf{r}'-\mathbf{r}'')\psi_s(\mathbf{r}')\psi_t(\mathbf{r}'')d\mathbf{r}'d\mathbf{r}'' , \quad (7)$$

respectively. The brackets [] in Eq. (5) denote antisymmetrization, i.e.,

$$[\langle mn|V|st \rangle] \equiv \langle mn|V|st \rangle - \langle mn|V|ts \rangle . \quad (8)$$

In Eq. (5), the indices a and b stand for hole states; their corresponding sums range over the core. The indices i and j stand for particle states; their corresponding sums range over all positive states outside the core.

Note that the expectation value of $\Sigma^{(2)}$,

$$\langle v|\Sigma^{(2)}|v \rangle = \sum_{a,i,j} \frac{1}{\varepsilon_v + \varepsilon_a - \varepsilon_i - \varepsilon_j} [\langle av|V|ij \rangle][\langle ij|V|av \rangle] + \sum_{a,b,i} \frac{1}{\varepsilon_v + \varepsilon_i - \varepsilon_a - \varepsilon_b} [\langle iv|V|ab \rangle][\langle ab|V|iv \rangle] , \quad (9)$$

is equal to the second-order correlation energy $E^{(2)}$ in perturbative calculation if $|v \rangle$ and ε_v are replaced by their DF counterparts.

We will call the second-order approximation the Brueckner approximation because the wave functions under this approximation are similar to the Brueckner orbitals used by others [9]. Equation (3) will be referred to the Brueckner equation, and its eigenfunctions and eigenvalues are accordingly called Brueckner wave functions and Brueckner energies, respectively.

B. Transition amplitudes

The transition amplitude in the hydrogenic approximation between the initial state $|n \rangle$ and the final state $|m \rangle$ is given by

$$u_{mn}(\omega) = \int \psi_m^{(0)\dagger}(\mathbf{r})(i\gamma_\mu)\psi_n^{(0)}(\mathbf{r})A_{\omega LM}^\mu(\mathbf{r})d\mathbf{r} , \quad (10)$$

where $\psi_m^{(0)}$ and $\psi_n^{(0)}$ are hydrogenic wave functions of states $|m \rangle$ and $|n \rangle$, respectively; γ_μ is the standard Dirac matrix and $A_{\omega LM}^\mu$ is the amplitude of the photon field with definite energy ω , angular momentum L , and projection M . Grant has shown that this transition amplitude is gauge invariant [10].

Intuitively, one would think the transition amplitude in the DF approximation is given by the right-hand side of Eq. (10) with the hydrogenic wave functions replaced by the DF wave functions. But numerical results show that this form of transition amplitude is not gauge invariant in the DF approximation. It was first discovered by Feldman and Fulton [11] that the gauge invariance of the transition amplitude in the DF approximation can be restored by adding a nonlocal contribution to the local form of Eq. (10). This nonlocal contribution comes naturally from the Green's-function formalism based on quantum electrodynamics. From the perturbative point of view, the nonlocal contribution is equivalent to the sum of a subset of all order contributions. Because the equation satisfied by the transition amplitude with the nonlocal contribution added is similar to a RPA equation [12], the nonlocal contribution is sometimes called the RPA-type contribution. Numerical results of the RPA-type

contribution show that they not only make transition amplitudes in the DF approximation gauge invariant, but also contribute substantially [7,13]. Thus any subsequent approximation should take the RPA-type contribution into consideration.

It is straightforward to extend the results of Feldman and Fulton [11] to the Brueckner approximation. In addition to the local form of Eq. (10), we have nonlocal contributions due to the first- and second-order kernels, $\Sigma^{(1)}$ and $\Sigma^{(2)}$. The transition amplitude between states $|m \rangle$ and $|n \rangle$ in the Brueckner approximation can be given as

$$\Lambda_{mn}(\omega) = u_{mn}(\omega) + Z_{mn}^{(1)}(\Lambda) + Z_{mn}^{(2)}(\Lambda) , \quad (11)$$

where u_{mn} is the local contribution given by Eq. (10) with the hydrogenic wave functions replaced by Brueckner wave functions. $Z_{mn}^{(1)}(\Lambda)$ is the RPA-type contribution. Explicitly, it can be written as [7]

$$Z_{mn}^{(1)}(\Lambda) = \sum_{a,i} \frac{1}{\varepsilon_n - \varepsilon_m + \varepsilon_a - \varepsilon_i} [\langle an|V|im \rangle] \Lambda_{ai}(\omega) + \sum_{a,i} \frac{1}{\varepsilon_m - \varepsilon_n + \varepsilon_a - \varepsilon_i} [\langle in|V|am \rangle] \Lambda_{ia}(\omega) , \quad (12)$$

which would be equivalent to the expression of first-order perturbative correction [Eq. (2) of Ref. [4]] if the nonlocal matrix elements Λ_{ai} and Λ_{ia} on the right-hand side are replaced by the local ones u_{ai} and u_{ia} , respectively. Let us denote the first-order perturbative correction by $Z_{mn}^{(1)}(u)$. $Z_{mn}^{(2)}(\Lambda)$ comes from photon insertions into $\Sigma^{(2)}$. Its explicit expression can be obtained from the expression of second-order perturbative corrections, $Z_{mn}^{(2)}(u)$, which is given in Eq. (4) of Ref. [4], by replacing all u_{st} with Λ_{st} . A diagrammatic representation of Eq. (11) is given in Ref. [4]. The transition amplitude $\Lambda_{mn}(\omega)$ can, in principle, be obtained by solving the set of self-consistent algebraic equations for all matrix elements $\Lambda_{st}(\omega)$. Without the term $Z_{mn}^{(2)}(\Lambda)$, Eq. (11) has exactly the form as in the DF approximation [13] and can easily be solved in the B -spline approximation as long as the Brueckner wave functions and energies have been ob-

TABLE I. Energy levels in the zeroth-, first-, and second-order approximations. The numbers in parentheses are percentage errors.

	State	Hydrogenlike	DF	Brueckner	Experiment ^a
Li	$2s_{1/2}$	-1.125 17	-0.196 32(0.9)	-0.197 98(0.1)	-0.198 14
	$2p_{1/2}$	-0.500 06	-0.128 64(1.2)	-0.130 03(0.2)	-0.130 24
	$2p_{3/2}$	-0.500 02	-0.128 64(1.2)	-0.130 03(0.2)	-0.130 23
Na	$3s_{1/2}$	-6.733 08	-0.182 03(3.6)	-0.188 38(0.2)	-0.188 86
	$3p_{1/2}$	-3.786 21	-0.109 49(1.9)	-0.111 37(0.2)	-0.111 60
	$3p_{3/2}$	-3.783 16	-0.109 42(1.9)	-0.111 29(0.2)	-0.111 52
K	$4s_{1/2}$	-11.325 67	-0.147 49(7.5)	-0.160 16(0.4)	-0.159 52
	$4p_{1/2}$	-7.243 78	-0.095 71(4.6)	-0.100 47(0.1)	-0.100 35
	$4p_{3/2}$	-7.229 74	-0.095 50(4.6)	-0.100 18(0.1)	-0.100 09
Rb	$5s_{1/2}$	-27.729 80	-0.139 29(9.3)	-0.155 00(1.0)	-0.153 51
	$5p_{1/2}$	-19.221 93	-0.090 82(5.6)	-0.096 57(0.4)	-0.096 19
	$5p_{3/2}$	-19.101 28	-0.089 99(5.4)	-0.095 44(0.3)	-0.095 11
Cs	$6s_{1/2}$	-43.067 96	-0.127 37(11.)	-0.146 42(1.8)	-0.143 10
	$6p_{1/2}$	-31.542 77	-0.085 62(7.1)	-0.093 19(0.9)	-0.092 17
	$6p_{3/2}$	-31.151 62	-0.083 78(6.5)	-0.090 39(0.7)	-0.089 64

^aReference [19].

tained from Eq. (3). The transition amplitude of the form given by Eq. (11) can be proven formally to be gauge invariant in the same way as in the case of the DF approximation [11].

III. NUMERICAL RESULTS AND DISCUSSIONS

Our object is to solve the Brueckner equation, Eq. (3), and then compute the dipole transition amplitudes, Eq. (11). Results of energies are given in atomic units. Results of transition amplitudes are given in their corresponding reduced matrix elements, also in atomic units.

To solve Eq. (3), we use the B -spline approximation [14] to generate a pseudospectrum of the complete set of orbitals. Thirty piecewise polynomials of order 7 are used as bases. First, the DF orbitals with angular momentum $l \leq 6$ are used in the right-hand side of Eq. (3) to get a new set of orbitals. This set of orbitals are then substituted into the right-hand side of Eq. (3) again. The process of iteration converges very fast. For the energy of the lowest valence state for each alkali-metal atom, taking the energy of the $5s$ state of Rb, for example, the results of the first and second iterations differ by 0.4%, and those of the second and third iterations differ by 0.04%. The use of the results of the second iteration should be acceptable for the accuracy we need. Notice that the term $\Sigma^{(2)}|\nu\rangle$ depends on the energy of state $|\nu\rangle$, ϵ_ν . We use the energy of the lowest valence state for each κ value [$\kappa = l(-l-1)$ if $j = l - \frac{1}{2}(l + \frac{1}{2})$] to generate the pseudospectrum. For example, in Cs we use ϵ_{6s} to generate 30 s orbitals, $\epsilon_{6p_{1/2}}$ to get 30 $p_{1/2}$ orbitals, and so on. This should be an acceptable approximation since the hole-state energies are present in the denominators of Eq. (5) and the expectation value of $\Sigma^{(2)}$ is several hundred times smaller than that of $\Sigma^{(1)}$.

Table I lists the energy of the three lowest valence states for each alkali-metal atom under zeroth-, first-, and second-order approximations. Dzuba *et al.* [6] have also tried to solve the Brueckner equation for the case of Cs. Their results for Brueckner energies are in better agreement with experimental values than ours. However, by comparing the results of the second-order correlation energy $E^{(2)}$, we see that our results are consistent with the results of Johnson, Idrees, and Sapirstein [5], while the results of Dzuba and co-workers [6,15] have a few percent discrepancy (Table II). Because the calculation of $E^{(2)}$ will result in the accuracy of Brueckner energies and wave functions, we thus believe their good agreement with experiment is fortuitous.

The Brueckner wave functions and energies obtained from Eq. (3) can now be used to compute transition amplitudes, Eq. (11). To obtain the gauge-invariant transition amplitudes, one has to solve the infinite set of coupled algebraic equations of all the matrix elements Λ_{st} . it is too complicated to be solved. We therefore first neglect the term $Z_{mn}^{(2)}(\Lambda)$ on the right-hand side of Eq. (11). The transition amplitudes under this approximation can be solved using the method described in Ref. [13]. The second-order contribution is then included by perturbation, namely, by adding the value of $Z_{mn}^{(2)}(u)$. The justification is as follows. By comparing perturbative results of photon insertions to $\Sigma^{(1)}$ and the RPA-type con-

TABLE II. Second-order correlation energy $E^{(2)}$ for Cs.

State	This work	Johnson <i>et al.</i> [5]	Dzuba <i>et al.</i> [6]
$6s_{1/2}$	-0.017 62	-0.017 75	-0.016 01
$6p_{1/2}$	-0.006 87	-0.006 91	-0.006 52
$6p_{3/2}$	-0.006 16	-0.006 18	-0.005 83

tributions, namely, $Z_{mn}^{(1)}(u)$ and $Z_{mn}^{(1)}(\Lambda)$, respectively (Table III), we see that these two values are of comparable size for all transitions; either the DF or Brueckner orbitals are used. We expect that the nonlocal contributions $Z_{mn}^{(2)}(\Lambda)$ will be close to the values of their corresponding perturbative results $Z_{mn}^{(2)}(u)$. Since $Z_{mn}^{(2)}(\Lambda)$ contributes very little to the transition amplitudes [0.02% (Li)–1.4% (Cs)], even if we had introduced 50% error in $Z_{mn}^{(2)}(\Lambda)$ by using $Z_{mn}^{(2)}(u)$, our final results for transition amplitudes would have only 0.01% (Li)–0.7% (Cs) error, which would not deteriorate the accuracy we expect for the Brueckner approximation. The length and velocity forms of our final results differ from each other by 0.02% (Li)–0.2% (Cs). Their average values are listed in column 8 of Table IV. Transition amplitudes in the zeroth- and first-order approximations are also listed in Table IV for comparison.

Our results for transition amplitudes in the Brueckner approximation differ from experimental values by 0.5% for the lightest atom (Li) and 1.2% for the largest one (Cs). Rubidium somehow has a larger error than cesium. This is not what one would expect since the accuracy of Brueckner energies for Rb are better than that for Cs (Table I). Except Rb, the accuracy is consistent with the accuracy of energy levels, where the percentage error ranges from 0.1% to 1.8% (see Table I).

The transition amplitudes under the Brueckner approximation are by no means the most accurate theoretical results. For Li, Weiss has done an extensive configuration-interaction calculation [16]. Blundell *et al.* have extended MBPT to an all-order calculation [17].

Their results for transition amplitudes are larger than experimental values by 0.4% and 0.3%, respectively. Blundell, Johnson, and Sapirstein have also reported their all-order calculation [18] for Cs. Their results are 4.525 (length) and 4.492 (velocity) for transition $6s \rightarrow 6p_{1/2}$, and 6.370 (length) and 6.328 (velocity) for $6s \rightarrow 6p_{3/2}$. These results differ from measured values by less than 0.5%. Nevertheless, the Brueckner approximation offers a systematic approach to all atoms or ions with a core plus one electron. It is accurate even for large atoms such as cesium (2% level of accuracy.) In addition, with the help of finite-basis methods, the numerical work is very simple.

IV. CONCLUSION

From a Green's-function formalism the hydrogenic, Dirac-Fock, and Brueckner approximations can be obtained systematically by cutting the kernel in Dyson's equation at zeroth, first, and second order, respectively, in electron-electron interactions. The transition amplitudes in these approximations can also be given in a gauge-invariant form. The energies and transition amplitudes in the Dirac-Fock approximation have been computed previously. In this paper we have used the *B*-spline method to solve for wave functions and energies and to compute the transition amplitudes in the Brueckner approximation. Compared with experimental values, energies have percentage error ranging from 1% to 11% in the Dirac-Fock approximation and 0.1% to 1.8% in the Brueckner approximation, increasing from Li to Cs.

TABLE III. Results of $Z^{(1)}(u)$, $Z^{(1)}(\Lambda)$, and $Z^{(2)}(u)$ using the DF and Brueckner orbitals.

Transition	DF orbitals			Brueckner orbitals				
	$Z^{(1)}(u)$	$Z^{(1)}(\Lambda)$	$Z^{(2)}(u)$	$Z^{(1)}(u)$	$Z^{(1)}(\Lambda)$	$Z^{(2)}(u)$		
Li	$2s_{1/2} \rightarrow 2p_{1/2}$	length	-0.012	-0.013	0.0006	-0.012	-0.014	0.0007
		velocity	-0.059	-0.080	-0.0004	-0.061	-0.083	-0.0004
	$2s_{1/2} \rightarrow 2p_{3/2}$	length	-0.016	-0.020	0.0009	-0.017	-0.020	0.0009
		velocity	-0.083	-0.112	-0.0005	-0.087	-0.118	-0.0006
Na	$3s_{1/2} \rightarrow 3p_{1/2}$	length	-0.038	-0.043	0.0028	-0.041	-0.047	0.0032
		velocity	-0.002	-0.004	0.0075	-0.003	-0.005	0.0082
	$3s_{1/2} \rightarrow 3p_{3/2}$	length	-0.054	-0.061	0.0040	-0.058	-0.066	0.0045
		velocity	-0.003	-0.005	0.0110	-0.003	-0.006	0.0116
K	$4s_{1/2} \rightarrow 4p_{1/2}$	length	-0.158	-0.144	0.017	-0.172	-0.166	0.019
		velocity	-0.020	-0.029	0.031	-0.025	-0.036	0.033
	$4s_{1/2} \rightarrow 4p_{3/2}$	length	-0.222	-0.217	0.024	-0.242	-0.234	0.026
		velocity	-0.026	-0.036	0.044	-0.033	-0.048	0.047
Rb	$5_{1/2} \rightarrow 5p_{1/2}$	length	-0.224	-0.213	0.027	-0.245	-0.231	0.030
		velocity	-0.028	-0.033	0.042	-0.036	-0.043	0.044
	$5s_{1/2} \rightarrow 5p_{3/2}$	length	-0.310	-0.297	0.036	-0.340	-0.321	0.041
		velocity	-0.030	-0.034	0.060	-0.041	-0.048	0.062
Cs	$6s_{1/2} \rightarrow 6p_{1/2}$	length	-0.334	-0.303	0.044	-0.372	-0.334	0.050
		velocity	-0.056	-0.062	0.062	-0.071	-0.078	0.062
	$6s_{1/2} \rightarrow 6p_{3/2}$	length	-0.453	-0.413	0.059	-0.498	-0.449	0.066
		velocity	-0.055	-0.050	0.087	-0.074	-0.076	0.088

TABLE IV. Transition amplitudes in zeroth-, first-, and second-order approximations. GI stands for "gauge invariant." The numbers in parentheses are percentage errors.

	Transition		Hydrogenlike	DF		Brueckner		Experiment
			(Local=GI)	Local	GI	Local	GI ^a	
Li	$2s_{1/2} \rightarrow 2p_{1/2}$	length	1.414	3.365	3.351	3.335	3.321	3.305 ^b
		velocity		3.430	(1.4)	3.404	(0.5)	
	$2s_{1/2} \rightarrow 2p_{3/2}$	length	2.000	4.759	4.739	4.717	4.696	4.674 ^b
		velocity		4.851	(1.4)	4.815	(0.5)	
Na	$3_{1/2} \rightarrow 3p_{1/2}$	length	0.943	3.690	3.647	3.584	3.540	3.513 ^b
		velocity		3.651	(3.8)	3.536	(0.8)	
	$3s_{1/2} \rightarrow 3p_{3/2}$	length	1.335	5.218	5.157	5.068	5.006	4.947 ^b
		velocity		5.162	(4.2)	4.999	(1.2)	
K	$4s_{1/2} \rightarrow 4p_{1/2}$	length	0.994	4.544	4.400	4.269	4.120	4.08 ^c
		velocity		4.429	(7.8)	4.122	(1.0)	
	$4s_{1/2} \rightarrow 4p_{3/2}$	length	1.409	6.439	6.222	6.035	5.825	5.77 ^c
		velocity		6.258	(7.8)	5.824	(0.9)	
Rb	$5s_{1/2} \rightarrow 5p_{1/2}$	length	0.800	4.819	4.606	4.440	4.237	4.11 ^d
		velocity		4.639	(12)	4.234	(3.2)	
	$5s_{1/2} \rightarrow 5p_{3/2}$	length	1.139	6.801	6.504	6.260	5.978	5.90 ^d
		velocity		6.538	(10)	5.961	(1.4)	
Cs	$6s_{1/2} \rightarrow 6p_{1/2}$	length	0.770	5.278	4.975	4.761	4.474	4.52 ^e
		velocity		5.037	(10)	4.488	(1.1)	
	$6s_{1/2} \rightarrow 6p_{3/2}$	length	1.101	7.426	7.013	6.674	6.286	6.36 ^e
		velocity		7.063	(10)	6.268	(1.2)	

^aThe values listed are actually the averages of the length and velocity forms. These two forms differ by less than 0.2%.

^bReference [20].

^cReference [21].

^dReference [22].

^eReference [23].

Transition amplitudes have percentage error ranging from 1.4% to 12% in the Dirac-Fock approximation and 0.5% to 1.2% in the Brueckner approximation (rubidium excluded.) Roughly speaking, the accuracy has been improved by one order of magnitude from the Dirac-Fock approximation to the Brueckner approximation. In addition, the energies and transition amplitudes have the same level of accuracy in either approximation.

The Brueckner approximation can be applied to all systems with a nondegenerate core plus one electron. In particular, one can take the core to be a closed subshell, such as in the case of boron and aluminum isoelectronic sequences. The correlation between the valence electron and the core is known to be much more important than it is in the case of alkali-metal atoms. The Brueckner approximation, having taken the second-order correlation into consideration, will be a much better model than

Dirac-Fock-approximation for these systems. Numerical work on these systems is currently under study.

One point that needs to be stressed is that the energies and transition amplitudes in each n th-order approximation based on the Green's-function formalism are gauge invariant. Also, corrections to the n th-order approximation can be calculated by perturbation. In particular, the corrections to the Brueckner approximation can be obtained by calculating perturbative contributions due to the third-order kernel. The computation is straightforward, but a great amount of CPU time is expected.

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- [1] S. S. Liaw, G. Feldman, T. Fulton, Phys. Rev. A **38**, 1126 (1988).
 [2] I. Lindgren and J. Morrison, *Atomic Many-Body Theory*, 2nd ed. (Springer-Verlag, Berlin, 1986).
 [3] S. A. Blundell, W. R. Johnson, and J. Sapirstein, Phys.

Rev. A **42**, 3751 (1991).

- [4] S. S. Liaw, Phys. Rev. A **47**, 1726 (1993).
 [5] W. R. Johnson, M. Idrees, and J. Sapirstein, Phys. Rev. A **35**, 3218 (1987).
 [6] V. A. Dzuba, V. V. Flambaum, P. G. Silvestrov, and O. P. Sushkov, J. Phys. B **18**, 597 (1985).

- [7] S. S. Liaw, *Can. J. Phys.* **70**, 1279 (1992).
- [8] Gy. Csanak, H. S. Taylor, and R. Yaris, *Adv. At. Mol. Phys.* **7**, 287 (1971).
- [9] See, for example, I. Lindgren, J. Lindgren, and A. M. Mårtensson, *Z. Phys. A* **279**, 113 (1976).
- [10] I. P. Grant, *J. Phys. B* **7**, 1458 (1974).
- [11] G. Feldman and T. Fulton, *Ann. Phys. (N.Y.)* **152**, 376 (1984); **172**, 40 (1986).
- [12] W. R. Johnson, C. D. Lin, K. T. Cheng, and C. M. Lee, *Phys. Scr.* **21**, 409 (1980).
- [13] S. S. Liaw, *Can. J. Phys.* **70**, 644 (1992).
- [14] W. R. Johnson, S. A. Blundell, and J. Sapirstein, *Phys. Rev. A* **37**, 307 (1988).
- [15] V. A. Dzuba, V. V. Flambaum, and O. P. Sushkov, *J. Phys. B* **16**, 715 (1983).
- [16] A. W. Weiss, *Can. J. Chem.* **70**, 456 (1992).
- [17] S. A. Blundell, W. R. Johnson, Z. W. Liu, and J. Sapirstein, *Phys. Rev. A* **40**, 2233 (1989).
- [18] S. A. Blundell, W. R. Johnson, and J. Sapirstein, *Phys. Rev. A* **43**, 3407 (1991).
- [19] C. E. Moore, *Atomic Energy Levels*, Natl. Bur. Stand. Ref. Data Ser., Natl. Bur. Stand. (U.S.) Circ. No. 35 (U.S. GPO, Washington, D.C., 1971) Vols. I–III.
- [20] A. Gaupp, P. Kuske, and H. J. Andrä, *Phys. Rev. A* **26**, 3351 (1982).
- [21] W. L. Wiese, M. W. Smith, and B. M. Miles, *Atomic Transition Probabilities—Sodium Through Calcium*, Natl. Bur. Stand. Ref. Data Ser., Natl. Bur. Stand. (U.S.) Circ. No. 22 (U.S. GPO, Washington, D.C., 1969), Vol. 2.
- [22] A. Gallagher and E. Lewis, *Phys. Rev. A* **10**, 231 (1974).
- [23] L. Shabanova, Yu. Monakov, and A. Khlyustalov, *Opt. Spektrosk.* **47**, 3 (1979) [*Opt. Spectrosc. (USSR)* **47**, 1 (1979)].