Mixed configuration-interaction and many-body perturbation-theory calculations of energies and oscillator strengths of $J=1$ odd states of neon

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Ab initio theory is developed for energies of $J=1$ particle-hole states of neutral neon and for oscillator strengths of transitions from such states to the $J=0$ ground state. Hole energies of low-Z neonlike ions are evaluated.

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I. INTRODUCTION

A combined configuration-interaction (CI) many-body-perturbation-theory (MBPT) method, applied previously to divalent atoms [1], is extended to particle-hole states of closed-shell atoms. After a derivation of CI+MBPT expressions for particle-hole states, we will apply the theory to calculations of energies and electric-dipole transition probabilities for neon.

For neon, many accurate measurements of transition rates are available, providing important tests of theory. Reciprocally, the theory might help to resolve existing discrepancies among oscillator strengths (f values) for transitions from the ground state to several excited states, for which experiments disagree. There is also a certain deficiency in existing *ab initio* theories in neon, for which discrepancies among many measurements and theoretical calculations are unsettled. For example, the only other elaborate *ab initio* calculations (Avgoustoglou and Beck [2]) gave an oscillator strength for the $[2p_{3/2}^{-1}3s_{1/2}]_1$ neon state, larger than most experimental values by more than two standard deviations. Extensive calculations performed by Hibbert *et al.* [3] for many transition rates along the neon isoelectronic sequence use a general configuration-interaction code (CIV3) [4]. The calculations utilized parametric adjustments with measured fine structures, but did not completely agree with experiments in neon and had an accuracy similar to other semiempirical calculations of Seaton [5]. However, the two calculations disagree with each other for several transitions. We hope that our calculations may help to understand better the theoretical problems in neon and provide guidance for the analysis of experimental data.

Some possible applications of the present CI+MBPT method include the study of the neonlike ions Si V, S VII, Ar IX, Ca XI, and Fe XVII that have astrophysical interest and have been included in the Opacity Project (Seaton [6]). The transition data in neon and other noble gases are also used in plasma physics, and in studying discharges that find many industrial applications in lamps and gas lasers. The methods presented here might be also used for improving the accuracy of MBPT or for extending the CI+MBPT method to more complicated open-shell atoms.

The principal theoretical difficulty arises from the sensitivity of transition amplitudes to the interaction between closely spaced fine-structure components. Although it is possible to obtain energies which are reasonably precise on an absolute scale using coupled-cluster methods (Ilyabaev and Kaldor [7]), accurate fine-structure splittings seem very difficult to obtain without semiempirical adjustments. This is why semiempirical approaches, which have fine-structure intervals carefully adjusted, are more successful in neon than are *ab initio* calculations. However, as we will demonstrate in this paper, CI calculations corrected with MBPT are also capable of accurately predicting fine-structure splittings and, consequently, transition amplitudes. In this paper, we will demonstrate the excellent precision of CI plus second-order MBPT. Third-order corrections, for which numerical codes already exist [8], can also be included, providing even further improvement in accuracy.

In Sec. II, we use the effective Hamiltonian formalism and particle-hole single-double coupled equations to derive expressions for the second-order Hamiltonian matrix of the CI+MBPT method. In the final expressions, we present a quite accurate MBPT that can predict energies of hole states and can appropriately describe the interactions in particle-hole atoms. The accuracy of hole energies obtained with the MBPT will be illustrated for neon and low-Z neon-like ions. Our CI+MBPT energies and f values for many states of neon are tabulated. Their agreement with experiment and other theories are shown.

II. CI+MBPT METHOD

The accuracy of the Rayleigh-Schrödinger variant of second-order MBPT, given in Ref. [9], is insufficient for our purpose, so that more accurate single-double equations must be used. The formulas for the correlation operator and a system of coupled equations for the correlation coefficients were given in Ref. [10]; we follow the notation of Ref. [10] in the paragraphs below. Under certain conditions, those equations can be further simplified and rewritten in the following forms:

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$$
\begin{aligned}
(\varepsilon_b-\varepsilon_\alpha)\chi_b^\alpha &= R_b^\alpha,\\
(\varepsilon_b+\varepsilon_c-\varepsilon_\alpha-\varepsilon_\beta-\tilde{g}_{bcbc})\chi_{bc}^{\alpha\beta} &= R_{bc}^{\alpha\beta}-\tilde{g}_{bcbc}\chi_{bc}^{\alpha\beta},\\
(\varepsilon_v-\varepsilon_r)\chi_v^r &= R_v^r,\\
(\varepsilon_a-\varepsilon_v)\chi_v^a &= R_v^a,\\
(\varepsilon_v+\varepsilon_b-\varepsilon_r-\varepsilon_s)\chi_{vb}^{rs} &= R_{vb}^{rs},\\
(\varepsilon_v+\varepsilon_b-\varepsilon_a-\varepsilon_s)\chi_{vb}^{as} &= R_{vb}^{as}.
\end{aligned}
\tag{1}
$$

In the second equation of this set, the term $\tilde{g}_{bcbc}\chi_{bc}^{\alpha\beta}$ is subtracted from both sides of this equation to make the right-hand side small. Since the large random-phase approximation (RPA) corrections in the particle-hole CI+MBPT are treated by CI, the quantities $W_{va'}^{v'a}$ entering this set of equations on the right-hand side in Ref. [10] are small, and have been neglected here. The concern might be raised for the correlation coefficients χ_{vb}^{as} and χ_v^r, which generally would have small factors $(\varepsilon_v+\varepsilon_b-\varepsilon_a-\varepsilon_s)$ or $(\varepsilon_v-\varepsilon_r)$ in front. However, for the large CI model space, energies of the core-virtual orbitals *bs* are well separated from the energies of the valence-hole orbitals *av*. The quantities R in zero approximation can be set to

$$
\begin{aligned}
R_j^i &= \Delta_{ij},\\
R_{bc}^{ij}-\tilde{g}_{bcbc}\chi_{bc}^{ij} &= g_{ijbc},\\
R_{vb}^{is} &= g_{isvb}
\end{aligned}
\tag{2}
$$

to obtain the first-order effective Hamiltonian

$$
H_{v'a',va}^{\mathrm{eff}} = (\varepsilon_v-\varepsilon_a)\,\delta_{v'v}\delta_{a'a}+H_{v'aa'v}^{(1)} \tag{3}
$$

and the correlation coefficients χ. Here we define the first-order correction $H_{v'aa'v}^{(1)}=\Delta_{v'v}\delta_{a'a}+\tilde{g}_{v'aa'v}$ to the effective Hamiltonian. For faster convergence of CI and for subtraction of the dominant monopole contributions in RPA diagrams, a $V^{(N-1)}$ Hartree-Fock (HF) model potential for which $\Delta_{nm}=\tilde{g}_{nama}$, $\Delta_{na}=\Delta_{an}=\Delta_{ab}=0$ is introduced.

Further improvement of accuracy can be achieved through iterations. After one iteration we obtain the second-order contribution to the effective Hamiltonian,

$$
H_{v'aa'v}^{(2)} = \delta R_v^{v'}\,\delta_{a'a}+\delta R_a^{a'}\,\delta_{v'v}+\delta\tilde{R}_{va}^{av'}, \tag{4}
$$

where

$$
\delta R_v^{v'} = \sum_{s\notin CI}\frac{\Delta_{v's}\Delta_{sv}}{\varepsilon_v-\varepsilon_s}-\sum_{scd}\frac{g_{cdvs}\tilde{g}_{v'scd}}{\varepsilon_c+\varepsilon_d-\varepsilon_{v'}-\varepsilon_s-\tilde{g}_{cdcd}}+\sum_{stc}\frac{g_{v'cst}\tilde{g}_{stvc}}{\varepsilon_v+\varepsilon_c-\varepsilon_s-\varepsilon_t}, \tag{5}
$$

$$
\delta R_a^{a'} = -\sum_{scd}\frac{g_{cda's}\tilde{g}_{ascd}}{\varepsilon_c+\varepsilon_d-\varepsilon_a-\varepsilon_s-\tilde{g}_{cdcd}}+\sum_{scd}\frac{g_{cda's}\tilde{g}_{ascd}}{\varepsilon_{a'}+\varepsilon_c-\varepsilon_s-\varepsilon_t-\tilde{g}_{a'ca'c}}, \tag{6}
$$

$$
\begin{aligned}
\delta\tilde{R}_{va}^{av'} = {}& \sum_{tu}\frac{g_{av'tu}\tilde{g}_{tuva'}}{\varepsilon_v+\varepsilon_{a'}-\varepsilon_t-\varepsilon_u}\\
&+\sum_{cd}\frac{\tilde{g}_{cdva'}g_{av'cd}}{\varepsilon_c+\varepsilon_d-\varepsilon_a-\varepsilon_{v'}-\tilde{g}_{cdcd}}+\sum_{t\notin CI}\frac{\tilde{g}_{av'ta'}\Delta_{tv}}{\varepsilon_v-\varepsilon_t}\\
&+\sum_{dt\notin CI}\frac{\tilde{g}_{dv'ta'}\tilde{g}_{atvd}}{\varepsilon_v+\varepsilon_d-\varepsilon_a-\varepsilon_t}\\
&-\sum_{dt}\frac{\tilde{g}_{dv'tv}\tilde{g}_{ata'd}}{\varepsilon_{a'}+\varepsilon_d-\varepsilon_a-\varepsilon_t-\tilde{g}_{a'da'd}}\\
&+\sum_{t\notin CI}\frac{\Delta_{v't}\tilde{g}_{taa'v}}{\varepsilon_v+\varepsilon_{a'}-\varepsilon_t-\varepsilon_a}\\
&+\sum_{dt}\frac{\tilde{g}_{datv}\tilde{g}_{v'ta'd}}{\varepsilon_{a'}+\varepsilon_d-\varepsilon_{v'}-\varepsilon_t-\tilde{g}_{a'da'd}}\\
&-\sum_{dt}\frac{\tilde{g}_{data'}\tilde{g}_{v'tvd}}{\varepsilon_v+\varepsilon_d-\varepsilon_{v'}-\varepsilon_t-\tilde{g}_{adad}}.
\end{aligned}
\tag{7}
$$

Note that in the last equation we have extended the single-double method. The last term entering $\delta\tilde{R}_{va}^{av'}$ in the single-double formalism would normally not contain $\tilde{g}_{adad}$ in the denominator. However, if we do not modify this denominator, we find that in the third-order MBPT, large terms proportional to $\tilde{g}_{adad}$ will appear leading to a decrease in accuracy. A physical reason for modifying the denominator of this term is that the process described by this term contains two holes in the intermediate states with large interaction energy. This interaction should be treated nonperturbatively, for example, by inclusion of $\tilde{g}_{adad}$ into the denominator as we have done on the basis of the single-double equations in other terms. Finally, this term is almost equal to the seventh term (they are complex conjugates and their Goldstone diagrams are related by a reflection through a horizontal axis), and for convenience they are set equal in numerical calculations. The angular reduction for $\delta\tilde{R}_{va}^{av'}$ can be easily obtained using the second-order particle-hole formulas given in Ref. [9].

III. A SOLUTION OF THE HOLE-ENERGY PROBLEM

A. Breit corrections

Apart from Coulomb correlation corrections, the Breit magnetic interaction is also important in neon and in the isoelectronic ions. The breakdown of various Coulomb and relativistic contributions to the energy of $3s$ states of neon was given in Ref. [10]. Breit corrections cancel, but for

TABLE I. A comparison of theoretical and experimental hole energies and the $2p_{3/2}$-$2p_{1/2}$ fine-structure intervals for neon and neonlike ions. All energies are in cm^{-1}.

	Ne	Na^+	Mg^{2+}	Al^{3+}	Si^{4+}
$2p_{3/2}$ Theor.	172434	380443	645951	967531	1344344
$2p_{3/2}$ Expt.	173930	381390	646402	967804	1345070
Difference	1496	947	451	273	726
$2p_{1/2}$ Theor.	173218	381816	648196	970997	1349449
$2p_{1/2}$ Expt.	174 710	382756	648631	971246	1350160
Difference	1492	940	435	249	711
$2p_{3/2}$-$2p_{1/2}$, Theor.	784	1373	2245	3466	5090
$2p_{3/2}$-$2p_{1/2}$, Expt.	780	1366	2229	3442	5105
Difference	−4	−7	−16	−24	−15

higher excited states they may not. Hence, to improve the accuracy of fine-structure splittings, we include the Hartree-Fock (HF) hole Breit correction $B_{aa}^{(\mathrm{HF})}$ in our calculations:

$$B_{aa}^{(\mathrm{HF})}=\sum_c \tilde{b}_{acca}. \tag{8}$$

We have checked that the first-order corrections $B^{(1)}$ to the energies of $J=2$ and 1 states given in Table I of Ref. [10] agree with our $B_{aa}^{(\mathrm{HF})}$ contributions, 0.00062 and 0.00090 a.u., for $2p_{3/2}$ and $2p_{1/2}$ states, respectively. We omit the small frequency-dependent Breit, quantum-electrodynamic, reduced-mass, and mass-polarization corrections. Small as they are, those corrections are further reduced after subtraction for the fine-structure intervals. More careful treatment of relativistic corrections is needed in calculations of high-Z neonlike ions.

B. Calculations of hole energies for neonlike ions

Since we propose a variant of the MBPT expansion, we would like first to demonstrate that this expansion is convergent for hole states. The theoretical hole energies shown in Table I have been obtained in the $V^{(N)}$ HF potential using Eq. (6) for δR_a^q to calculate second-order corrections. The extra term in the denominator is important and is necessary for convergence of the perturbation expansion. Experimental hole energies in the National Institute of Standards and Technology (NIST) database Ref. [11] are found as the limit energies for the neon isoelectronic sequence. For neutral neon only one limit, the $p_{3/2}$ energy is given in NIST [11]. The $2p_{1/2}$-$2p_{3/2}$ splitting 780.4269(36) cm^{-1} was measured in Ref. [12], and using this value we find the experimental $p_{1/2}$ energy. Table I demonstrates the good agreement of our theoretical $p_{3/2}$, $p_{1/2}$ energies as well as the same fine structure interval for neon-like ions. Our fine-structure interval, whose correctness is crucial for transition amplitude calculations, differs from experiment just by about 10 cm^{-1}. Note that the HF value 187175 cm^{-1} for the $2p_{3/2}$ state is 8.5% higher than the experimental value 173930 cm^{-1}, and, after adding correlation corrections, we obtain improvement by a factor of 10. For the fine structure, the HF value 1001 cm^{-1} disagrees even more, by 28%. If we use Rayleigh-Schrödinger perturbation theory, the corrections are twice as large as our results, and the agreement with experiment does not improve.

TABLE II. A comparison with experiment of CI+MBPT energies referenced to the ground state and given in atomic units. An almost constant shift is subtracted in the fifth column to demonstrate excellent agreement for relative positions of levels.

Level	Experiment	CI+MBPT	Δ	Δ − 0.0069
$p_{3/2}^{-1}3s$	0.6126	0.6048	0.0078	0.0009
$p_{1/2}^{-1}3s$	0.6192	0.6116	0.0076	0.0007
$p_{3/2}^{-1}4s$	0.7235	0.7166	0.0070	0.0001
$p_{1/2}^{-1}4s$	0.7269	0.7200	0.0069	0.0000
$p_{3/2}^{-1}3d$	0.7360	0.7289	0.0070	0.0001
$p_{3/2}^{-1}3d$	0.7365	0.7294	0.0071	0.0002
$p_{1/2}^{-1}3d$	0.7401	0.7330	0.0071	0.0002
$p_{3/2}^{-1}5s$	0.7560	0.7491	0.0069	0.0000
$p_{1/2}^{-1}5s$	0.7593	0.7525	0.0069	0.0000

IV. NEON ENERGIES AND OSCILLATOR STRENGTHS OF $J=1$ ODD STATES

To test the accuracy of the CI+MBPT method, we first calculated energies of several lowest odd $J=1$ neon states (Table II). The number of configurations in CI was chosen to be 52. The order of eigenstates obtained in the CI+MBPT method is the same as the order of the experimental levels. We abbreviate long NIST designations since the levels are uniquely specified by energy or by order.

The pure *ab initio* energies differ from experimental energies by 0.0069 a.u., but after subtraction of the systematic shift (which does not make much difference in transition calculations), the agreement is at the level of 0.0001 a.u. for almost all states. Therefore, we consider the accuracy of the CI+MBPT method adequate for a correct prediction of level mixing and oscillator strengths. For the $3s$ states, agreement with experiment for the fine structure interval is much better than that obtained by Avgoustoglou *et al.* [10], 0.0002 versus

TABLE III. Our CI+MBPT oscillator strengths for the ground to excited state transitions in neon compared with average experimental values (third and fourth columns) and those obtained with the best semiempirical theories [3,5,13].

Levels	CI+MBPT	σ avr.	Mean	Ref. [5]	Ref. [13]	Ref. [3]
$p_{3/2}^{-1}3s$	0.0102	0.0099	0.0107	0.0126	0.0106	0.0123
$p_{1/2}^{-1}3s$	0.1459	0.1549	0.1487	0.1680	0.1410	0.1607
$p_{3/2}^{-1}4s$	0.0131	0.0122	0.123	0.0152	0.0124	
$p_{1/2}^{-1}4s$	0.0181	0.0170	0.016	0.0193	0.0160	
$p_{3/2}^{-1}3d$	0.0066			0.0056	0.0045	0.0047
$p_{3/2}^{-1}3d$	0.0130	0.0187	0.0199	0.0167	0.0131	0.0117
$p_{1/2}^{-1}3d$	0.0069	0.0067	0.0069	0.0086	0.0064	0.0055
$p_{3/2}^{-1}5s$	0.0068	0.0064	0.0066	0.0073	0.0060	
$p_{1/2}^{-1}5s$	0.0053	0.0043	0.0044	0.0050	0.0043	

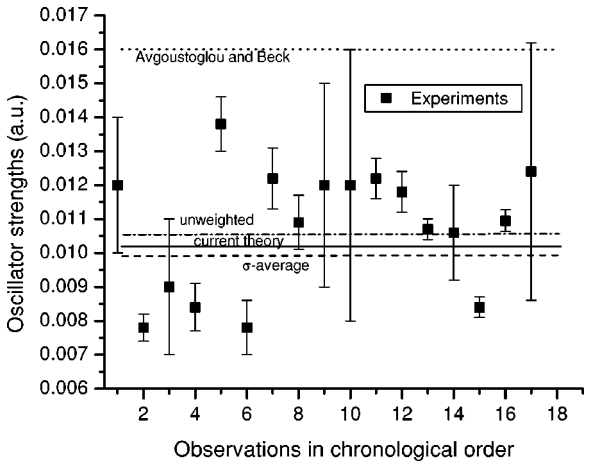

FIG. 1. Comparison with experiment for oscillator strengths of the $[p_{3/2}^{-1}3s]_1$ state of neon.

0.0012 a.u.; a possible explanation for this could be that single-double equations miss important corrections which we included by modifying the denominators. In Ref. [10], however, the systematic shift is small.

Finally, we present our CI+MBPT oscillator strengths in neon. After a diagonalization of the second-order effective Hamiltonian, we obtain wave functions in the form of expansion coefficients in the CI space and use them to calculate oscillator strengths. Size-consistent formulas for dipole matrix elements for transitions decaying into the ground state were provided in Ref. [2], where the absorption oscillator strength f is also defined. In Table III we give *ab initio* values of the oscillator strengths f. The dominant part of the RPA corrections is included at the level of CI. Small normalization corrections are omitted.

Many experiments have disagreements in oscillator strengths far exceeding the cited errors (see Fig. 1 and Table IV): hence, for comparison, in Table III we give two statistical averages: the first is a weighted according to cited standard deviations and the second is an unweighted average. For the $3s$ levels, the experimental data compiled in Ref. [2] and for the higher excited levels in Ref. [29] have been included in the averaging. Average values obtained here are not necessarily the most accurate, but they serve well for comparison and for a test of our probably less accurate calculated values.

A more careful analysis of experimental techniques to exclude systematic errors, which are definitely present, is necessary; our values can provide some guidance. For $p_{3/2}^{-1}3d$ states, since the energy separation of the two states is small, experiments give the sum of the two oscillator strengths, and the value 0.0196 rather than 0.0130 should be compared with the experimental values 0.0187 (0.0199). In Table III, we also compare our theory with other semiempirical theories. Surprisingly, early calculations by Aleksandrov *et al.* [13] agreed well with our calculations. A fair agreement, considering the high sensitivity of these transitions to correlation correction, is also obtained with the other theories in Table III.

TABLE IV. References for experimental data shown in Fig. 1.

Obs.	Reference	Year	f	σ
1	Kuhn *et al.* [14]	1967	0.01200	0.00200
2	Lawrence and Liszt [15]	1969	0.00780	0.00040
3	Geiger [16]	1970	0.00900	0.00200
4	Kernahan *et al.* [17]	1971	0.00840	0.00070
5	Kazantsev and Chaika [18]	1971	0.01380	0.00080
6	Knystautas and Drouin [19]	1974	0.00780	0.00080
7	Bhaskar and Luro [20]	1976	0.01220	0.00090
8	Westerveld *et al.* [21]	1979	0.01090	0.00080
9	Aleksandrov *et al.* [13]	1983	0.01200	0.00300
10	Chornay *et al.* [22]	1984	0.01200	0.00400
11	Tsurubuchi *et al.* [23]	1990	0.01220	0.00060
12	Chan *et al.* [24]	1992	0.01180	0.00060
13	Ligtenberg *et al.* [25]	1994	0.01070	0.00030
14	Suzuki *et al.* [26]	1994	0.01060	0.00140
15	Curtis *et al.* [27]	1995	0.00840	0.00030
16	Gibson and Risley [28]	1995	0.01095	0.00032
17	Zhong *et al.* [29]	1997	0.01240	0.00380

V. CONCLUSIONS

In this paper, we have introduced a CI+MBPT method for particle-hole states of closed-shell atoms. A difficulty that the hole energy has poor convergence is overcome with modifications of denominators in MBPT. Good precision for hole states and for particle-hole states is illustrated for many energy levels of neon. Apart from energies, our theory is tested in calculations of oscillator strengths. Agreement with averaged experimental values is achieved.

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