V^{N-M} approximation for atomic calculations

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We demonstrate that V^{N-M} approximation is a good starting point for the configuration interaction calculations for many-electron atoms and ions. N is the total number of electrons in the neutral atom, M is the number of valence electrons. V^{N-M} is the self-consistent Hartree-Fock potential for a closed-shell ion with all valence electrons removed. Using of the V^{N-M} approximation considerably simplifies the many-body perturbation theory for the core-valence correlations. It makes it easier to include higher-order correlations which often significantly improves the accuracy of the calculations. Calculations for krypton and barium and their positive ions are presented for illustration.

I. INTRODUCTION

Atomic physics is a valuable tool to study many fundamental problems. It is used to study parity and time invariance violating interactions (see, e.g. [1]), possible variation of the fundamental constants in quasar absorption spectra [2] and in present-day experiments by comparing the rates of different atomic clocks [3], etc. However, interpretation of the atomic measurements is often limited by accuracy of atomic calculations. For example, the accuracy of the most precise measurements of atomic parity nonconserving effects (PNC) in atoms which has been achieved for cesium is 0.35% [4]. The accuracy of the best calculations is from 0.5 to 1% [5–8]. The situation is even worse for thallium. Experimental accuracy of the PNC measurements is 1% [9] while best theoretical accuracy is from 2.5% [10] to 3% [11]. On this level of accuracy there is perfect agreement of the PNC measurements with the standard model and any further progress would need significant improvement in atomic theory. There are many other examples where accurate atomic calculations are needed. These include atomic clocks, quantum computations, plasma physics, etc. Therefore, it is worth to study the ways of improving the methods of calculations.

It is well known that the perturbation theory in residual Coulomb interaction converge very poorly for many electron atoms and some all-order technique is needed to achieve good accuracy of calculations. For atoms with one external electron above closed shells there are at least two all-order methods which lead to a fraction of percent accuracy in calculation of the energies as compared to experimental data. One is an all-order correlation potential method (also called perturbation theory in screened Coulomb interaction) [12]. Another is linearized coupled cluster approach (CC) [13]. For atoms with more than one external electron good accuracy can be achieved when different methods are combined to include correlations between valence electrons together with the core-valence correlations. This can be done by combining configuration interaction method with the many-body

perturbation theory (CI+MBPT) [14] or CC method with the MBPT [15] or with the CI method [16].

The key question in developing of all these methods is where to start or what potential to chose to generate a complete set of single-electron states. It is well accepted now that the Hartree-Fock potential is the best choice for the perturbation theory expansion. This is because self-consistency condition leads to exact cancellation between Coulomb and potential terms in the residual interaction so that potential terms are completely eliminated from the perturbation theory expansion. The natural choice for atoms with one external electron is the V^{N-1} Hartree-Fock potential introduced by Kelly [17]. In the V^{N-1} approximation the self-consistency procedure is initially done for a closed-shell positive ion. States of external electron are then calculated in the field of frozen core. There is exact cancellation between direct and exchange self-action terms in the Hartree-Fock potential for closed shell systems. Therefore, by including self-action, we can easily see that states in the core and states above core are calculated in the same potential. Other words, V^{N-1} potential generates a complete set of orthogonal single-electron states which are convenient for use in the perturbation theory expansion. Using this set in an appropriate all-order method leads to very good results for a neutral atom in spite of the fact that the core of the atom is actually the core of a positive ion.

The V^{N-1} approximation can also be used for atoms with more than one external electron. However, in this case the system of $N-1$ electrons is most likely to be an open-shell system and some averaging procedure is needed to define the V^{N-1} potential. Another complication arise when core-valence correlation are to be included by means of MBPT. There is no exact cancellation between potential terms any more. The potential in the effective Hamiltonian is now V^{N-M} potential, where M is number of valence electrons and $M > 1$. Perturbation theory expansion would have terms proportional to $V^{N-M} - V^{N-1}$. These terms are called *subtraction diagrams* [14] or Δ *terms* [18]. The number of these terms is larger than number of pure Coulomb terms and this represents significant complication of the MBPT. These terms can be totally avoided if calculations from the very beginning are done in the V^{N-M} potential. However, it is widely believed

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TABLE I. Parameters of core states of Kr I and Kr IX (atomic units).

State	Energy	$\langle r \rangle$	$\langle r^2 \rangle^{1/2}$	$r(f_{\max})$	$f_{\max}$	r_1	r_2
			Kr I				
$1s$	−529.6849	0.0415	0.0481	0.0269	4.3707	0.0151	0.0731
$2s$	−72.0798	0.1827	0.1986	0.1541	2.4630	0.0987	0.2839
$2p_{1/2}$	−64.8748	0.1574	0.1744	0.1216	2.4476	0.0731	0.2605
$2p_{3/2}$	−62.8792	0.1613	0.1784	0.1253	2.4283	0.0753	0.2605
$3s$	−11.2245	0.5271	0.5648	0.4704	1.5508	0.3182	0.7794
$3p_{1/2}$	−8.6199	0.5314	0.5744	0.4577	1.4924	0.3006	0.7996
$3p_{3/2}$	−8.3128	0.5412	0.5848	0.4704	1.4800	0.3093	0.8202
$3d_{3/2}$	−3.7776	0.5505	0.6095	0.4098	1.3459	0.2681	0.9072
$3d_{5/2}$	−3.7268	0.5543	0.6136	0.4098	1.3415	0.2681	0.9072
$4s$	−1.1877	1.6008	1.7136	1.3629	0.8954	0.9535	2.4031
$4p_{1/2}$	−0.5415	1.9147	2.0711	1.5253	0.7921	1.1037	2.9420
$4p_{3/2}$	−0.5143	1.9586	2.1196	1.5594	0.7825	1.1037	2.9942
			Kr IX				
$1s$	−534.8482	0.0415	0.0481	0.0269	4.3708	0.0151	0.0731
$2s$	−77.1131	0.1827	0.1985	0.1541	2.4633	0.0987	0.2839
$2p_{1/2}$	−69.9296	0.1573	0.1743	0.1216	2.4480	0.0731	0.2605
$2p_{3/2}$	−67.9321	0.1613	0.1783	0.1253	2.4288	0.0753	0.2605
$3s$	−16.1190	0.5258	0.5630	0.4704	1.5530	0.3182	0.7794
$3p_{1/2}$	−13.5239	0.5285	0.5706	0.4577	1.4970	0.3006	0.7996
$3p_{3/2}$	−13.2140	0.5378	0.5805	0.4704	1.4851	0.3093	0.8202
$3d_{3/2}$	−8.6967	0.5376	0.5918	0.4098	1.3624	0.2605	0.8628
$3d_{5/2}$	−8.6450	0.5411	0.5955	0.4098	1.3584	0.2681	0.8848

that doing calculations for a neutral atom by starting from a highly charged ion would lead to poor convergence of the perturbation expansion and poor end results. Indeed, after the initial Hartree-Fock procedure is done the core is kept frozen in all consequent calculations. No further perturbation expansion can change anything in the core, leaving it to be the core of the highly charged ion.

The purpose of this work is to demonstrate that the core of the highly charged ion is often not very much different from the core of neutral atom and V^{N-M} approximation can be a good approximation for atoms with several valence electrons. The main gain is total elimination of subtraction diagrams. This significantly simplifies the perturbation theory expansion for the core-valence correlations. It is also much easier to include higher-order core-valence correlations in the V^{N-M} approximation. Inclusion of higher-order correlations can significantly improve the accuracy of the calculations.

We consider CI+MBPT calculations for neutral krypton and barium and their positive ions to illustrate the advantage of the V^{N-M} approximation.

II. CALCULATIONS

A. Krypton

Let us start our consideration from an extreme case - an atom with eight valence electrons. The purpose of this ex-

ample is to illustrate that even removal of as many as eight electrons do not lead to any dramatic changes in the atomic core and V^{N-8} approximation is still reasonably good approximation for the neutral atom as well as for the all chain of positive ions starting from number of valence electrons $M=1$ and up to $M=8$.

Table I compares core states of Kr I and Kr IX. Calculations are done in V^N and V^{N-8} potentials, respectively. We present singe-electron energies, overage radius ($\langle r \rangle$), square root of overage square radius ($\langle r^2 \rangle^{1/2}$), position of the maximum of the wave function ($r(f_{\max})$), the value in the maximum ($f_{\max}$) as well as the range of distances where 80% of the electron density is located (from r_1 to r_2). It is easy to see that changing from V^N to V^{N-8} potential has large effect on the energies of core states but not on their wave functions. Indeed, the energy of $3d$ states change almost two times while overage radius (or square root of overage square radius) changes by about 2–3 % only, position of the maximum does not change at all and the value of the wave function in the maximum changes by about 1% only.

To understand this behavior one should look at the distances where electrons are localized. As can be seen from Table I valence electrons ($4s$ and $4p$) are localized at significantly larger distances than core electrons. There is almost no overlap between densities of core and valence electrons. Indeed, 90% of the density of the $4s$ and $4p$ electrons are at distances $r > a_B$ ($0.95 a_B$ for the $4s$ state and $1.1 a_B$ for the $4p$ state) while 90% of the density of the uppermost core state
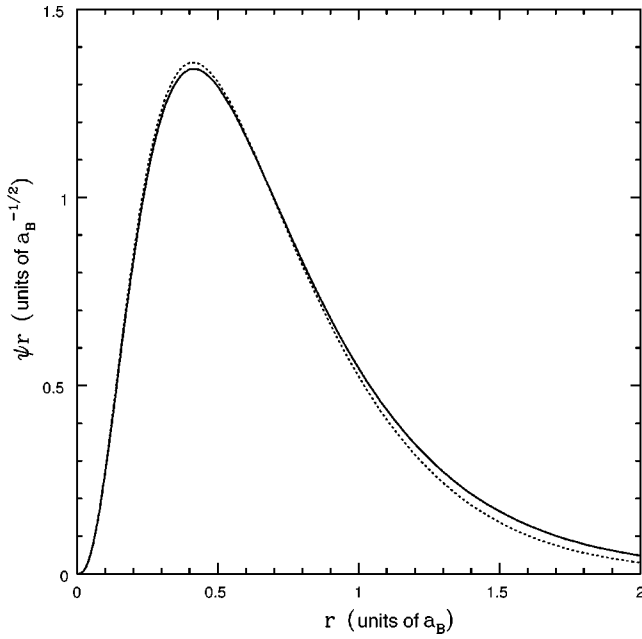
FIG. 1. Radial wave function of the $3d_{5/2}$ state of Kr I (solid line) and Kr IX (dotted line).

$3d$ is at $r < 0.907 a_B$. This means that valence states can only create constant field inside the core. For example,

$$Y_{0(4s)}(r) = \int \frac{|\psi_{4s}(r')|^2}{r_>} dr' \approx \text{const at } r < a_B.$$

Correction to the energy of a core state is given by diagonal matrix element

$$\delta\epsilon_n \sim \int |\psi_n(r)|^2 Y_0(r) dr.$$

This matrix element is large.

In contrast, correction to wave function is given by off-diagonal matrix elements. These matrix elements are small due to orthogonality of wave functions:

$$\int \psi_n(r)^\dagger \psi_m(r) Y_0(r) dr \approx \text{const} \int \psi_n(r)^\dagger \psi_m(r) dr = 0.$$

Figure 1 shows the $3d_{5/2}$ radial wave functions of Kr I and Kr IX. One can see that they are almost identical. There is some difference at large distances due to different energies $[\psi \sim \exp(-\sqrt{2|\epsilon|}r)]$. This difference has some effect on the normalization of the wave function leading to small difference in the maximum. Apart from this the wave functions are very similar.

We see that the removal of eight valence electrons from Kr I affects only energies of the core states but not their wave functions. Obviously, change in the energies affects the MBPT for the core-valence correlations through the change in energy denominators. But what is more important is the absence of the subtraction diagrams which makes the MBPT to be much more simple. Excitation energies are larger in Kr IX than in Kr I which means that MBPT terms are smaller and convergence is likely to be better. Therefore, it is natural

TABLE II. Energy levels of Kr VIII (cm^{-1}).

State	HF	Brueckner	Expt.[a]
$4s$	1004870	1015504	1014665
$4p_{1/2}$	862612	871429	870970
$4p_{3/2}$	852990	861472	861189
$4d_{3/2}$	635048	640449	640618
$4d_{5/2}$	633695	639065	639284

[a]NIST, [19].

to assume that the V^{N-8} approximation is a good initial approximation for all krypton ions starting from Kr IX and up to neutral Kr I, with number of valence electrons ranges from none to eight. We have performed the calculations to check this.

Hartree-Fock energy of the $3d_{5/2}$ state of Kr IX (8.645 a.u., see Table I) agrees within 2% with the experimental ionization energy of Kr IX (8.488 a.u. [19]). The difference should be mostly attributed to the correlations.

We can do much better calculations for Kr VIII. It has one valence electron above closed shells. We calculate its states in the field of frozen core (V^{N-8} potential) in Hartree-Fock and Brueckner approximations. The latter means that we modify the HF equations for valence electron by including correlation potential $\hat{\Sigma}$ (see [20] for details). We calculate $\hat{\Sigma}$ in second order of MBPT. The results are presented in Table II. As can be seen Hartree-Fock energies differ from experiment by about 1% while inclusion of correlations improves them significantly brining the agreement to better than 0.1%.

We use the combined CI+MBPT method for ions with more than one valence electron [14]. Like in standard CI method the Schrödinger equation is written for the many-electron wave function of valence electrons

$$(\hat{H}^{\text{eff}} - E)\Psi = 0. \tag{1}$$

Ψ has a form of expansion over single-determinant many-electron wave functions

$$\Psi = \sum_i c_i \Phi_i(r_1, \ldots, r_M). \tag{2}$$

Ψ_i are constructed from the single-electron valence basis states calculated in the V^{N-M} potential. E in (1) is the valence energy (energy needed to remove all valence electrons from the atom).

The effective Hamiltonian has the form

$$\hat{H}^{\text{eff}} = \sum_{i=1}^{M} \hat{h}_{1i} + \sum_{i \neq j}^{M} \hat{h}_{2ij}, \tag{3}$$

$\hat{h}_1(r_i)$ is the one-electron part of the Hamiltonian

$$\hat{h}_1 = c\alpha\mathbf{p} + (\beta - 1)mc^2 - \frac{Ze^2}{r} + V^{N-8} + \hat{\Sigma}_1. \tag{4}$$

$\hat{\Sigma}_1$ is the second-order correlation potential which was used for Kr VIII.

$\hat{h}_2$ is the two-electron part of the Hamiltonian

TABLE III. Ground state removal energies of Kr VIII to Kr I (a.u.).

	State		Expt.[a]	Calc.
Kr VIII	$4s$	$^2S_{1/2}$	−4.62317	−4.62699
Kr VII	$4s^2$	$^1S_0$	−8.70247	−8.64060
Kr VI	$4s^24p$	$^2P^o_{1/2}$	−11.58709	−11.52481
Kr V	$4s^24p^2$	$^3P_0$	−13.96459	−13.89050
Kr IV	$4s^24p^3$	$^4S^o_{3/2}$	−15.89375	−15.74736
Kr III	$4s^24p^4$	$^3P_2$	−17.25163	−17.03929
Kr II	$4s^24p^5$	$^2P^o_{3/2}$	−18.14684	−17.88392
Kr I	$4s^24p^6$	$^1S_0$	−18.66132	−18.28761

[a]NIST, [19].

$$\hat{h}_2 = \frac{e^2}{|\mathbf{r}_1 - \mathbf{r}_2|} + \hat{\Sigma}_2(r_1, r_2), \qquad (5)$$

$\hat{\Sigma}_2$ is the two-electron part of core-valence correlations. It represents screening of Coulomb interaction between valence electrons by core electrons. We also calculate $\hat{\Sigma}_2$ in the second order of MBPT. The details of the calculation of $\hat{\Sigma}_1$ and $\hat{\Sigma}_2$ can be found elsewhere [14,21]. Note however that in contrast to the cited works we now have no subtraction diagrams.

Only number of electrons changes in the effective Hamiltonian (3) when we move from Kr VII ($M=2$) to Kr I ($M=8$) while terms V^{N-8}, $\hat{\Sigma}_1$, and $\hat{\Sigma}_2$ remain exactly the same.

The results for ground state energy of removal all valence electrons are compared with experiment in Table III. Accuracy of calculations for all ions and neutral atom are similar and always better than 2%.

To compare the V^N and V^{N-8} approximations we have also performed calculations of the ground state energy of Kr I in V^N potential with the same size of the basis set and with core-valence correlations included in the second order of MBPT (including subtraction diagrams). The result is −18.377 a.u. which differs by only 0.5% from the result obtained in V^{N-8} potential and by 1.5% from the experiment.

B. Atoms with two valence electrons

The fact that V^{N-2} approximation works well for atoms like Mg, Ca, Ba, etc. is pretty well known (see, e.g., Ref. [22]). In this section we demonstrate that inclusion of the higher than second-order core-valence correlations can lead to further significant improvements in accuracy of atomic calculations. It is much easier to include higher-order correlations in the V^{N-2} approximation than in any other potential.

We consider barium atom as an example and start calculations from Ba II. Table IV presents HF and Brueckner energies of Ba II together with the experimental values. Brueckner energies are calculated with the second-order correlation potential $\hat{\Sigma}^{(2)}$ and with the all-order correlation potential $\hat{\Sigma}^{(\infty)}$. The all-order $\hat{\Sigma}^{(\infty)}$ includes screening of Coulomb interaction and hole-particle interaction (see, e.g. [12]).

TABLE IV. Energy levels of Ba II (cm^{-1}).

State	HF	$\hat{\Sigma}^{(2)}$	$\hat{\Sigma}^{(\infty)}$	Expt.[a]
$6s$	75339	82318	80816	80687
$6p_{1/2}$	57265	61180	60603	60425
$6p_{3/2}$	55873	59388	58879	58734
$5d_{3/2}$	68139	77224	76345	75813
$5d_{5/2}$	67665	76286	75507	75012

[a]NIST, [19].

Similar to what happens for alkali atoms, inclusion of higher-order correlation corrections for Ba II reduces the difference between theoretical and experimental energies from 1–2% to 0.2–0.7%.

Now we are going to use the same correlation potential $\hat{\Sigma}_1$ for the neutral barium. The effective Hamiltonian has the form similar to (3)

$$\hat{H}^{\text{eff}} = \hat{h}_1(r_1) + h_1(r_2) + \hat{h}_2(r_1, r_2). \qquad (6)$$

One-electron part $\hat{h}_1$ is given by Eq. (4); two-electron part $\hat{h}_2$ is given by Eq. (5). For the operator $\hat{\Sigma}_1$ in (4) we use second-order correlation potential $\hat{\Sigma}^{(2)}$ and all-order correlation potential $\hat{\Sigma}^{(\infty)}$, the same as for the Ba II ion.

We do not include higher-order correlations in $\hat{\Sigma}_2$ in present work. Formally, perturbation expansion for both $\hat{\Sigma}$ goes over the same orders of MBPT. However, calculations show that accurate treatment of $\hat{\Sigma}_1$ is usually more important. Since the aim of present work is to demonstrate the advantages of the V^{N-M} approximation rather than presenting best possible calculations, neglecting higher-order correlations in $\hat{\Sigma}_2$, which has small effect on final results, is justified.

Table V shows the results of calculations for few low states of Ba I in the V^{N-2} approximation with $\hat{\Sigma}^{(2)}$ and $\hat{\Sigma}^{(\infty)}$ together with the experimental data. One can see that inclusion of the higher-order core-valence correlations do indeed improve significantly the agreement between theoretical and experimental data.

It is interesting to note that there is strong correlation between results for Ba I and Ba II. In both cases the least accurate results are for states involving d electrons. Inclusion of higher-order core-valence correlations leads to very similar improvement of results for Ba II and Ba I. Also, if $\hat{\Sigma}_1$ is rescaled to fit the experimental energies of Ba II, the agreement between theory and experiment for Ba I would also be almost perfect. This feature can be used to get very accurate results for negative ions. Experimental results for negative ions are poor and accurate calculations are difficult. However, if we start calculations from the V^{N-M} approximation, include $\hat{\Sigma}$ for core-valence correlations, rescale $\hat{\Sigma}_1$ to fit known energies of a positive ion or neutral atom, the results for a negative ion are also going to be very accurate.

TABLE V. Two-electron removal energies of Ba I (a.u.).

State		Expt.[a]	$\hat{\Sigma}^{(2)}$	$\Delta(\%)$[b]	$\hat{\Sigma}^{(\infty)}$	$\Delta(\%)$[b]
$6s^2$	$^1S_0$	−0.559152	−0.569963	1.9	−0.559032	0.02
$6s5d$	$^3D_1$	−0.517990	−0.529157	2.2	−0.520645	0.67
	$^3D_2$	−0.517163	−0.528203	2.1	−0.519799	0.51
	$^3D_3$	−0.515423	−0.526182	2.1	−0.518029	0.51
	$^1D_2$	−0.507231	−0.516504	1.8	−0.508819	0.31
$6s6p$	$^3P_0$	−0.503264	−0.510328	1.4	−0.502636	0.12
	$^3P_1$	−0.501575	−0.508609	1.4	−0.500983	0.12
	$^3P_2$	−0.497574	−0.504472	1.4	−0.497013	0.11
	$^1P_1$	−0.476863	−0.485072	1.7	−0.478031	0.24
$5d6p$	$^3F_2$	−0.458618	−0.466239	1.7	−0.461060	0.53
	$^3F_3$	−0.454596	−0.461833	1.6	−0.456956	0.52
	$^3P_4$	−0.450906	−0.457765	1.5	−0.453187	0.51

[a]NIST, [19].
[b]$\Delta = |E_{calc} - E_{expt}| / |E_{expt}| \times 100\%$.

C. Atoms with more than two valence electrons

We have demonstrated that V^{N-M} approximation works very well for atoms with two and eight valence electrons. In is natural to expect that there are many similar cases in between.

However, there is no reason to believe that this approximation works well for all atoms. There are many cases were it does not work at all. It depends mostly on the distances where valence electrons are located rather than on their number. To check whether the V^{N-M} approximation is a good approximation for a neutral atom it is usually sufficient to perform Hartree-Fock calculations for this atom and check that valence electrons are localized on larger distances than core electrons. This is usually the case if valence electrons are in s or p states. In contrast, d and f valence electrons are localized on distances shorter than the distances of the uppermost core s and p electrons. Their removal would lead to significant change in the atomic core which means that the V^{N-M} approximation is not good for these atoms.

Roughly speaking, the V^{N-M} approximation should work more or less well for about half of the Periodic Table.

III. CONCLUSION

We have demonstrated that the V^{N-M} approximation in which initial Hartree-Fock procedure is done for an ion with all valence electrons removed, is a good starting point for accurate calculations for many-electron atoms with s and/or p valence electrons. The main advantage is relatively simple MBPT for core-valence correlations which makes it easier to include higher-order core valence correlations and thus improve the accuracy of the calculations.

Considering examples of Kr and Ba we have demonstrated that removal of as many as eight electrons from initial HF potential does not compromise the accuracy of the calculations for a neutral atom and that inclusion of the higher-order core-valence correlations do really lead to significant improvements of the accuracy of the calculations.

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