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Electronic structure of Li$^-$ and F$^-$ calculated directly in momentum space

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Summary. A self-consistent field method is applied to compute directly in momentum space the electronic structures of the bound anions Li$^-$ and F$^-$ at the Hartree–Fock level. The convergence towards the Hartree–Fock limit, starting from STO-3G, 3-21G, 3-21+G and 6-311+G AO's, is stable and monotonous. Substantial improvement in the quality of the anion orbitals is noted already after one iteration. Particularly interesting is the efficiency with which the method modifies and improves the shape of the trial functions.

Key words: Momentum space – Atomic Hartree–Fock orbital – Gaussian basis set – Asymptotic properties of the wave function – Li anions – F anions

1 Introduction

Stable (or bound) anions are species that lie energetically below the ground state of their parent neutral [1, 2]. Their outermost orbitals correspond to diffuse electron densities, orbital energies close to the ionization limit, and low average values of kinetic energy. A theoretical description of isolated atomic and molecular anions requires special care (level of theory, large basis sets, etc.) that is not usually needed for the corresponding neutral and cationic species. The Hartree–Fock (HF) model, for example, often predicts anions that are not stable compared to the neutral atom, which points to the need for correlation corrections. However, within the conventional LCAO-MO scheme, the limitation of the atomic basis sets is by far the most significant source of error, which reflects the inherent difficulty of describing the diffuse nature of the electron density of anionic species. To perform accurate calculations on anions, large basis sets are constructed by supplementing the valence atomic basis sets with diffuse [3, 4] or floating [5] atomic functions. The construction of such bases is often performed using sequences of even tempered basis functions [6].

The momentum space approach [7–9] has proved to possibly bring improvements in the description of the basis sets used for anions. As a matter of fact, the momentum and direct-space functions and equations are related by a Fourier transform and contain the same information, but express it differently.

For instance, in momentum space the emphasis is put on the valence part of the electronic structure [10] since diffuse orbitals in position space which have in momentum space most of their amplitude concentrated around the origin. In an exact scheme this has no effect on the results, while in an approximate treatment it can be used advantageously for a better description of the valence region, which is precisely where problems arise in the case of anionic species [11].

Attempts to solve the HF equations for atoms [7, 12–16] and small molecules [8, 9, 17–19] directly in momentum space have shown definite improvements on the resulting wave functions. Considering the importance of good atomic and molecular orbitals, and thus basis sets, for post-Hartree–Fock treatments we study in this paper the improvements brought by a direct momentum space scheme on the wave functions of four- (Li^-) and ten- (F^-) electron ions. From these specific applications, we tentatively draw some general considerations about calculations on anions in momentum space. A brief summary on the momentum space closed-shell atomic HF equations and the momentum space SCF scheme is given in the next section.

2 SCF momentum space method

In momentum space, the closed-shell atomic HF equations describing a m-electron atom of nuclear charge Z writes, in atomic units, as:

$$\begin{aligned}\frac{p^2}{2}\phi_i(p) - \frac{Z}{2\pi^2}\int\frac{dq}{q^2}\phi_i(p-q) + 2\sum_{j=1}^{m/2}\frac{1}{2\pi^2}\int\frac{dq}{q^2}W^*_{jj}(q)\,\phi_i(p-q)\\ - \sum_{j=1}^{m/2}\frac{1}{2\pi^2}\int\frac{dq}{q^2}W^*_{ij}(q)\,\phi_j(p-q) = \varepsilon_i\,\phi_i(p), \quad i = 1,2,\cdots m/2. \qquad (1)\end{aligned}$$

ε_i stands for the orbital energy of the ith momentum-space orbital $\phi_i(p)$. And $W_{i,j}(q)$, the convolution product of $\phi_i(p)$ and $\phi_j(p)$, is defined as:

$$W_{ij}(q) = \int dp\,\phi^*_i(p)\,\phi_j(p-q). \qquad (2)$$

As in position space, the solution of the HF equations in momentum space requires an iterative procedure which basically includes four steps:

Step 1. Initialization of the procedure.
A set of trial functions is chosen, and the corresponding orbital energies are calculated directly in momentum space:

$$\varepsilon_i = \int dp\,\phi^*_i(p)\,[F\phi_i](p), \quad i = 1,2,\cdots m/2. \qquad (3)$$

$[F\phi_i](p)$ stands for the left-hand side of the momentum space HF equation, Eq. (1).

Step 2. Iteration of the wavefunction.
When functions and energies are known for the kth iteration, the functions at the next iteration are obtained according to a method originally proposed by Lassettre [7] and Navaza–Tsoucaris [8] (a detailed description of the method can be found in Ref. [20]), but modified to deal with non-bound states,

$$\phi_i^{(k+1)}(p) = \left[\frac{p^2}{2} - E_i^{(k)}\right]^{-1}\left\{\int dq\,V_{ij}^{(k)}(q)\,\phi_i^{(k)}(p-q) + C\phi_i^{(k)}(p)\right\}, \qquad (4)$$

where $V_{ij}^{(k)}(q)\phi_i^{(k)}(p-q)$ stands for the left-hand side of Eq. (1), the kinetic term excepted.

A translation of the energy origin is performed by fixing C positive in the next expression:

$$E_i^{(k)} = \varepsilon_i^{(k)} - C, \tag{5}$$

to avoid singularities in the $[p^2/2 - E_i^{(k)}]$ term when the orbital energies $\varepsilon_i^{(k)}$ are either positive (corresponding to non-bound states) or too close to zero. In all other cases, C is zero. The orbitals are reorthonormalized after each iteration.

Explicit calculations through first iteration, $k = 1$ in Eq. (4), are not only possible with gaussians, but also relatively simple. This, in particular, allows to use trial orbitals $\phi_i^{(0)}(p)$ coming from standard quantum chemistry packages and introduce them directly in the iterative scheme. Unfortunately, the transcendental functions in terms of which the $\phi_i^{(1)}(p)$ are expressed at the end of the first iteration (especially the convolution product) do not lead to closed-form expressions for these integrals and a numerical procedure is therefore needed. This constitutes a barrier to carry out further iterations to improve the orbitals by approaching the HF limit. In order to carry out further iterations, we propose a compromise between a fully numerical scheme and the simple first iteration approach. The scheme is based on the fact that at the end of each iteration the $\phi_i^{(k)}(p)$'s entail the main qualitative characteristics of the exact solution and most importantly the right asymptotic decay. The idea is thus to fit the iterated analytical functions $\phi_i^{(k)}(p)$ obtained at the kth step on a finite set of gaussian functions (a set of nine gaussians allows a satisfactory fit with low variance about 10^{-7}) and then use these fitted functions as a new set of trial functions $\phi_i^{g(k)}(p)$. The advantage is twofold. First, with exponents and linear coefficients specific for each orbital, energies and functions are quickly improved. Second, the problematic convolution products and integrals are efficiently computed in terms of the gaussian functions obtained to represent the $\phi_i^{g(k)}(p)$'s. At the end of the whole process, properties which do not include convolution products in their expression (e.g. $\langle p^{-1}\rangle$, $\langle p\rangle$, $\langle p^2\rangle$, etc.) are obtained by direct numerical integration of the last iterated orbitals $\phi_i^{(k)}(p)$ to benefit from the functional characteristics imparted by the momentum-space iteration. The details of the analytical and numerical steps involved in the momentum-space procedure are given in Ref. [21].

Step 3. Calculation of energies of the iterated functions.
The orbital energies are calculated in momentum space using Eq. (3).

Step 4. End of iterations.
Step 2 and 3 are repeated until a given convergence (energy, physical property or mean-squared deviation between successive iterated functions) threshold is reached.

3 Results and discussion

In their ground states, Li$^-$ and F$^-$ are both closed-shell atomic negative ions, with $1s^2 2s^2$ and $1s^2 2s^2 2p^6$ singlet electronic configurations, respectively. The atomic orbitals of Li$^-$ and F$^-$ are computed according to the momentum-space SCF procedure described above, trial functions are obtained from the Gaussian 90 program [22].

Table 1. Starting with trial functions (0) expressed in standard basis sets of increasing quality, a first iteration (1) is performed for Li^-. The atomic orbital properties are given in atomic units, and to help comparison near HF limits [23, 24] are reported

	1s			2s				
Li^- iteration	$\langle p^{-1}\rangle$	$\varepsilon_{\mathrm{kin}}$	ε	$\langle p^{-1}\rangle$	$\varepsilon_{\mathrm{kin}}$	ε	E_T	Vi
STO-3G								
0	0.66059	7.0260	− 1.9686	3.1212	0.80691	+ 0.10225	− 7.2133	− 1.9209
1	0.66444	6.9447	− 2.2307	4.3811	0.31916	+ 0.01547	− 7.4086	− 2.0200
3-21G								
0	0.65864	7.1418	− 2.2384	4.6021	0.30107	+ 0.00643	− 7.3668	− 1.9898
1	0.65320	7.1215	− 2.3188	5.6920	0.20543	− 0.01077	− 7.4270	− 2.0137
3-21 + G								
0	0.65502	7.1427	− 2.2958	6.3672	0.23659	− 0.01401	− 7.3769	− 1.9997
1	0.65829	7.1257	− 2.3320	6.5552	0.19833	− 0.01477	− 7.4266	− 2.0140
6-311 + G								
0	0.65660	7.2232	− 2.3213	6.2869	0.20505	− 0.01422	− 7.4275	− 1.9999
1	0.65655	7.2243	− 2.3238	6.4914	0.20135	− 0.01497	− 7.4282	− 2.0003
[23]	0.65644	7.2261	− 2.3228	6.4347	0.20216	− 0.01453	− 7.4282	− 2.0000
[24]	–	7.2261	− 2.3228	–	0.20215	− 0.01454	− 7.4282	− 2.0000

In order to assess the orbital quality over a large domain of momentum, some physical properties of the orbitals $\phi_i^{(k)}(p)$ are computed at each iteration k. They are the orbital energies $\varepsilon_i (i = 1s, 2s$ or $2p)$, total energy (E_T), kinetic energies $\varepsilon_{\mathrm{kin},i} (i = 1s, 2s$ or $2p)$, Virial ratio (Vi) which measures the overall quality of the orbitals, and the $\langle p^{-1}\rangle_i (i = 1s, 2s$ or $2p)$ terms which probe preferentially the region of low momenta:

$$\langle p^{-1}\rangle_i = \int dp\, \phi_i^*(p) \left[\frac{1}{p}\right] \phi_i(p). \tag{6}$$

The AO's computed in direct space with the Gaussian 90 program for the standard STO-3G, 3-21G, 3-21+G and 6-311+G bases are then used as trial functions in a one-momentum space iteration. The corresponding physical properties are compared with the near HF values calculated with the STO expansion of Clementi and Roetti [23] expressed in momentum space, and those calculated with the numerical direct-space SCF program of Froese Fischer [24]. All quantities being listed in Tables 1 and 2, respectively for Li^- and F^-. The near HF values for the anions reflect significantly more diffuse charge densities for the valence ($2s$ and $2p$) orbitals than for the parent neutral [23]. Indeed, the valence orbitals of Li^- and F^- have low orbital energies, low average values of kinetic energy and high values of the $\langle p^{-1}\rangle$ term.

As seen in Tables 1 and 2, it is only when diffuse functions are included in the basis sets that satisfactory values are obtained with the LCAO-SCF scheme. This because the iterative procedure based on the variational principle selects coefficients that ensure the lowest possible total energy out of the available degrees of freedom. It is also due to the fact that the exponents in the standard bases have been tailored to the neutral species and are not optimal for the anion. The minimal

Table 2. Starting with trial functions (0) expressed in standard basis sets of increasing quality, a first iteration (1) is performed for F$^-$. The atomic orbital properties are given in atomic units, and to help comparison near HF limits [23, 24] are reported

	1s			2s			2p				
F$^-$ iteration	$\langle p^{-1} \rangle$	ε_{kin}	ε	$\langle p^{-1} \rangle$	ε_{kin}	ε	$\langle p^{-1} \rangle$	ε_{kin}	ε	E_T	Vi
STO-3G											
0	0.20136	73.174	− 24.706	0.98375	7.6517	− 0.59974	0.53273	6.4960	+ 0.37319	− 97.613	− 1.9731
1	0.20181	72.715	− 25.395	1.0833	7.1481	− 0.97309	0.70913	6.5203	− 0.10048	− 99.039	− 1.9955
3-21G											
0	0.20073	73.804	− 25.437	1.0278	7.7158	− 0.88525	0.60376	5.9004	+ 0.00586	− 98.772	− 1.9955
1	0.20166	73.563	− 25.692	1.0635	7.6068	− 1.0433	0.73235	6.0297	− 0.16238	− 99.338	− 1.9988
3-21+G											
0	0.20131	73.812	− 25.741	1.0716	7.7969	− 1.0752	0.72367	5.5717	− 0.18434	− 98.934	− 2.0062
1	0.20156	73.590	− 25.827	1.0681	7.8009	− 1.0718	0.72164	5.6452	− 0.18243	− 99.365	− 2.0087
6-311+G											
0	0.20066	74.503	− 25.827	1.0672	7.4450	− 1.0702	0.71296	5.7248	− 0.17737	− 99.446	− 2.0002
1	0.20107	74.298	− 25.828	1.0649	7.7757	− 1.0728	0.72704	5.7238	− 0.18023	− 99.458	− 1.9998
[23]	0.20064	74.507	− 25.830	1.0677	7.7689	− 1.0744	0.72383	5.7277	− 0.18085	− 99.459	− 2.0000
[24]	-	74.507	− 25.830	-	7.7697	− 1.0746	-	5.7277	− 0.18099	− 99.460	− 2.0000

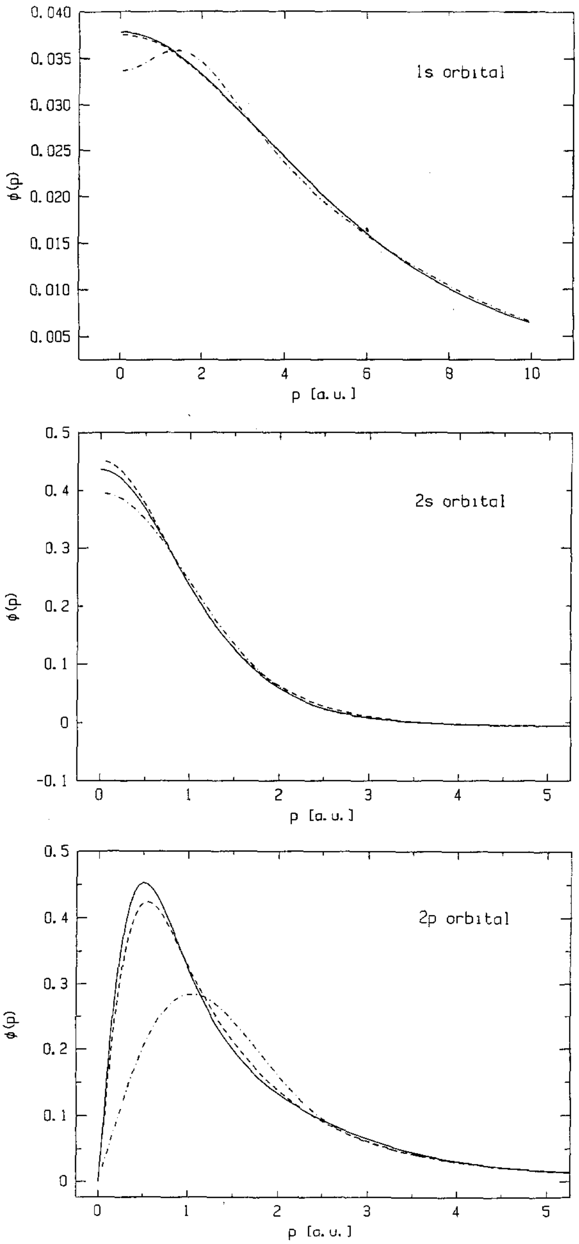

Fig. 1. Graphs, with respect to the modulus of the momentum (p), of the atomic orbitals of F^- after one iteration (——). The graphs of the trial function (·—·—), expressed in the 3-21G basis, and of the near Hartree–Fock limit function [23] (– – – –) are added to appreciate the improvement brought by the iteration

STO-3G basis [25] gives very poor results, even from a qualitative point of view since the outermost orbital leads to a positive eigenvalue or a non-bound state. The split-valence 3-21G basis [26] does not change the picture significantly, whereas significant improvements are observed with the 3-21+G basis [4] which includes diffuse functions. It might be worth adding that the 3-21+G basis, which yields results comparable to the 4-31+G basis [3], was in fact optimized on the singlet ground states of first row anions, and thus on Li^- and F^-. Results close to the near HF limit are obtained with the very good diffuse split valence 6-311 + G basis [4].

One momentum-space iteration results in dramatic improvements, as can be read in Tables 1 and 2 and seen in Fig. 1. Even if the trial functions are expressed in the rather limited STO-3G and 3-21G bases, a nearly correct description of the bound nature of the outermost orbitals is obtained after one single iteration. The improvements occur in both core and valence levels, but the most significant changes are imparted to the valence orbitals. The orbital energies are always corrected in the right direction, whatever the energy level and/or the ion. For instance, ε_{2p}(3-21 + G) of F^-, too low in energy (– 0.18434 au), is corrected to – 0.18243 au after one iteration. Similarly, ε_{2p}(6-311 + G) of Li^-, too high in energy (– 0.01422 au), is corrected to – 0.01497 au again after one iteration. It must also be stressed that these variations occur for quite small changes in energies in the case of the more extended bases as well as for larger variations for the small bases. That the corrections always go in the right directions is also observed for the other properties. The graphs in Fig. 1 emphasize the qualitative importance of the changes imposed on the behaviour of the 3-21G atomic orbitals of F^- after a single iteration. In the case of the 1*s* orbital, the momentum space treatment corrects the peculiar behaviour near the origin [16] and, even though it is not apparent on the graph, forces the right $|p|^{-4}$ asymptotic decay for $\phi_{1s}(p)$ at large momentum [12, 19, 27]. This correction is responsible for the strong energy improvement in both the ε_{1s} and E_T energies. In the case of the 2*s* one-electron state, the amplitude of $\phi_{2s}(p)$, too low near the origin, is enhanced, but slightly in excess. The most dramatic improvement is shown in the case of the $\phi_{2p}(p)$ orbital which after one iteration has its maximum not only enlarged but also shifted towards low momentum. As can be seen in the graphs, the behaviour of the three functions is much affected and always in the right direction. These graphs also show how valuable momentum space is to assess the quality of the valence orbitals of which essential features are concentrated in a rather limited interval of momentum values around the origin, while in direct space they tail off exponentially over large distances [28, 29].

Table 3. Convergence towards the HF limits of the atomic orbital properties (in a.u.) of Li^-. The trial functions are expressed in the STO-3G basis set, and to help comparison near HF limit results [23, 24] are reported

	1*s*			2*s*				
Li^- iteration	$\langle p^{-1}\rangle$	ε_{kin}	ε	$\langle p^{-1}\rangle$	ε_{kin}	ε	E_T	*Vi*
0	0.66059	7.0260	– 1.9686	3.1212	0.80691	0.10225	– 7.2133	– 1.9209
1	0.66444	6.9447	– 2.2306	4.3811	0.31916	0.01621	– 7.4096	– 2.0201
2	0.65965	7.1083	– 2.2898	5.2055	0.23075	– 0.00318	– 7.4255	– 2.0118
3	0.65765	7.1801	– 2.3162	5.8646	0.20442	– 0.01210	– 7.4282	– 2.0060
4	0.65690	7.2079	– 2.3197	6.0597	0.20300	– 0.01329	– 7.4282	– 2.0024
5	0.65663	7.2188	– 2.3213	6.2448	0.20248	– 0.01393	– 7.4282	– 2.0010
6	0.65651	7.2237	– 2.3217	6.2849	0.20230	– 0.01424	– 7.4282	– 2.0003
7	0.65649	7.2244	– 2.3219	6.3613	0.20223	– 0.01438	– 7.4282	– 2.0001
8	0.65648	7.2248	– 2.3223	6.3622	0.20219	– 0.01440	– 7.4282	– 2.0000
[23]	0.65644	7.2261	– 2.3228	6.4347	0.20216	– 0.01453	– 7.4282	– 2.0000
[24]	–	7.2261	– 2.3228	–	0.20215	– 0.01454	– 7.4282	– 2.0000

Table 4. Convergence towards the HF limits of the atomic orbital properties (in a.u.) of F$^-$. The trial functions are expressed in the STO-3G basis set, and to help comparison near HF limit results [23, 24] are reported

	1s			2s			2p				
F$^-$ iteration	$\langle p^{-1}\rangle$	ε_{kin}	ε	$\langle p^{-1}\rangle$	ε_{kin}	ε	$\langle p^{-1}\rangle$	ε_{kin}	ε	E_T	Vi
0	0.20136	73.174	− 24.706	0.98375	7.6517	− 0.59974	0.53273	6.4960	+ 0.37319	− 97.613	− 1.9731
1	0.20181	72.715	− 25.395	1.0833	7.1481	− 0.97309	0.70913	6.5203	− 0.10048	− 99.039	− 1.9955
2	0.20115	73.256	− 25.649	1.0951	7.2254	− 1.0013	0.69891	6.1333	− 0.12928	− 99.397	− 2.0061
3	0.20111	73.647	− 25.781	1.0921	7.3830	− 1.0534	0.71732	5.9087	− 0.17243	− 99.437	− 2.0054
4	0.20102	73.913	− 25.826	1.0831	7.5300	− 1.0687	0.72164	5.7861	− 0.18184	− 99.448	− 2.0051
5	0.20090	74.108	− 25.833	1.0760	7.6357	− 1.0721	0.72274	5.7424	− 0.18196	− 99.453	− 2.0035
6	0.20079	74.244	− 25.828	1.0717	7.7058	− 1.0721	0.72367	5.7316	− 0.18039	− 99.454	− 2.0017
[23]	0.20064	74.507	− 25.830	1.0677	7.7689	− 1.0744	0.72383	5.7277	− 0.18085	− 99.459	− 2.0000
[24]	–	74.507	− 25.830	–	7.7697	− 1.0746	–	5.7277	− 0.18099	− 99.460	− 2.0000

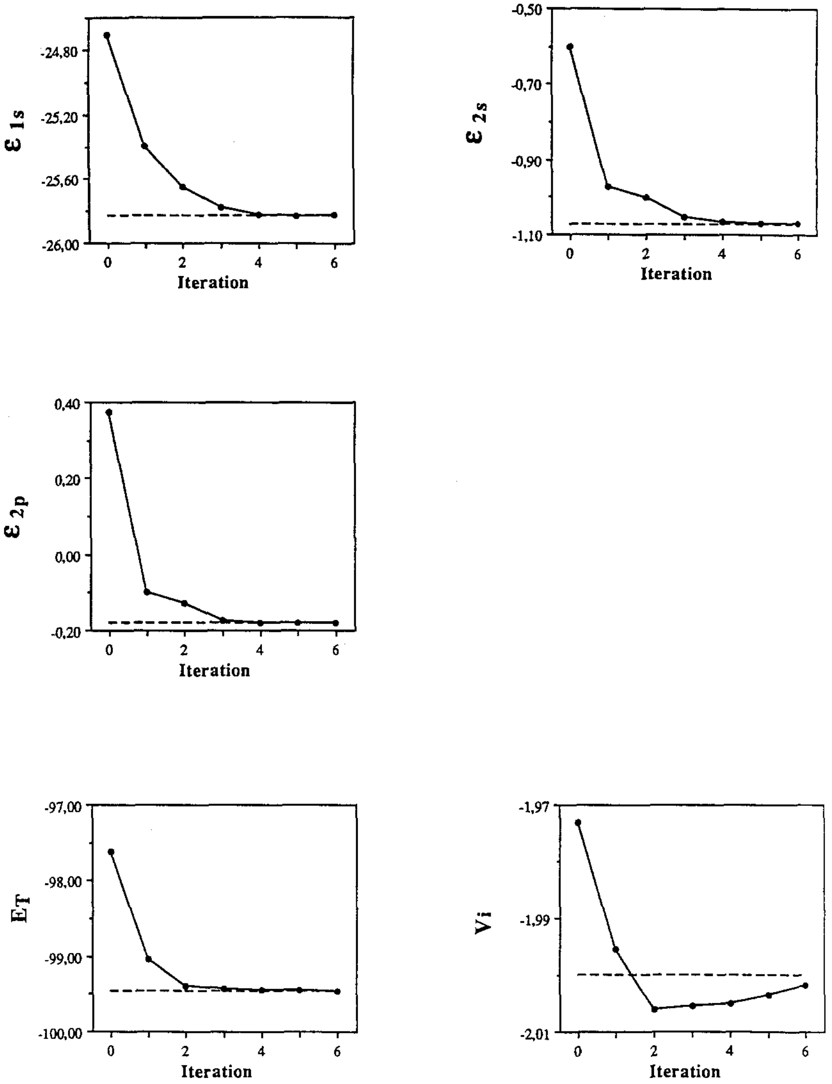

Fig. 2. Convergence towards the near HF limits [23] (represented by *dotted lines*) of the energetical properties (in a.u.) of F$^-$. The trial functions are expressed in the STO-3G basis set

The orbital characteristics of Li$^-$ and F$^-$ at each iteration of the momentum-space SCF scheme starting with the STO-3G basis are reported in Tables 3 and 4, respectively. The evolutions during the iterations of the energy parameters ε_{1s}, ε_{2s}, ε_{2p}, E_T and the Virial ratio for F$^-$ are plotted in Fig. 2. It is obvious that the corrections are stable, follow a monotonous convergence pattern and the largest changes occur during the first four iterations.

4 Conclusions

The momentum space SCF method tested on Li$^-$ and F$^-$ seems to be well suited to deal with anions. The convergence towards the HF limit is stable and monotonous, and a first iteration already improves significantly the quality of the orbitals initially represented with usual Gaussian basis sets (such as the minimal STO-3G or the diffuse double-zeta 3-21 + G). Furthermore, the special view the momentum space provides on orbitals, especially the valence functions, is another strong motivation for developing an algorithm to calculate the electronic structure of atoms and molecules directly in momentum space. Work is now in progress to apply the momentum-space SCF method to bound molecular anions.

References

1. Radom L (1977) in: Schaefer III HF (ed) Application of electronic structure theory. Plenum Press, NY, chap 8
2. Simons J, Jordan KD (1987) Chem Rev 87:535
3. Chandrasckhar J, Andrade JG, Schleyer PvR (1981) J Am Chem Soc 103:5609
4. Clark T, Chandrasckhar J, Spitznagel GW, Schleyer PvR (1983) J Comput Chem 4:294
5. Helgaker T, Almlöf J (1988) J Chem Phys 89:4889
6. Cooper DL, Wilson S (1982) J Chem Phys 77:4551
7. Huo WM, Lassettre EN (1980) J Chem Phys 72:2374
8. Navaza J, Tsoucaris G (1981) Phys Rev A 24:683
9. Berthier G, Defranceschi M, Delhalle J (1989) in: Defranceschi M, Delhalle J (eds) Numerical Determination of the Electronic Structure of Atoms, Diatomic and Polyatomic Molecules', NATO-ASI, Vol C271. Kluwer Acad, Dordrecht, p 209
10. Cooper DL, Allan NL (1992) J Am Chem Soc 114:4773
11. Ishida T, Ohno K (1989) Int J Quantum Chem 35:257
12. Delhalle J, Fripiat JG, Defranceschi M (1987) Ann Soc Scient Brux 101:9
13. Delhalle J, Fripiat JG, Defranceschi M (1990) Bull Soc Chim Belg 3:135
14. Defranceschi M, Delhalle J (1990) Eur J Phys 11:172
15. De Windt L, Fripiat JG, Delhalle J, Defranceschi M (1991) Ann Soc Scient Brux 105:89
16. De Windt L, Fripiat JG, Delhalle J, Defranceschi M (1992) J Mol Stuct (Theochem) 254:145
17. Defranceschi M, Suard M, Berthier G (1984) Int J Quantum Chem 25:863
18. Alexander SA, Coldwell RL, Monkhorst HJ (1988) J Comp Phys 76:263
19. Fischer P, Defranceschi M, Delhalle J (1992) Numer Math 63:67
20. De Windt L, Delhalle J, Defranceschi M (1993) Int J Quantum Chem 45:609
21. De Windt L, Delhalle J, Defranceschi M, Fischer P, Fripiat JG, 'A combined analytical and numerical strategy to solve the atomic Hartree–Fock equations in momentum space', to be published
22. Gaussian90, Revision F (1990) Frisch MJ, Head–Gordon M, Trucks MJ, Foresman J, Schlegel HB, Raghavachari K, Robb M, Binkley JS, Gonzalez C, Defrees DJ, Fox DJ, Whiteside DA, Seeger R, Melius CF, Baker J, Martin RL, Kahn LR, Stewart JJP, Topiol S, Pople JA, Gaussian Inc Pittsburgh PA
23. Clementi E, Roetti C (1974) Atomic Data Nucl Data Tables 14:177
24. Froese Fischer C (1986) Comput Phys Rep 3:273
25. Hehre WF, Stewart RF, Pople JA (1969) J Chem Phys 51:2657
26. Binkley JS, Pople JA, Hehre WJ (1980) J Am Chem Soc 102:939
27. Benesch R, Smith VH (1973) in: Chissick SS, Ravensdale T (eds) Wave mechanics, the first fifty years. Butterworth, London, chap 21
28. Handy NC, Marron MT, Silverstone HJ (1969) Phys Rev 180:45
29. Hoffman–Ostenhof M, Hoffman–Ostenhof T (1977) Phys Rev A 16:1782