IC/90/381

INTERNATIONAL CENTRE FOR
THEORETICAL PHYSICS

ON THE POSSIBILITY OF LOCALIZING OF ELECTRON GROUP FUNCTIONS USING THE NOTION OF ANTISYMMETRICAL ORTHOGONALITY

Vladimir E. Puchin

and

Boris P. Zapol

INTERNATIONAL
ATOMIC ENERGY
AGENCY

UNITED NATIONS
EDUCATIONAL,
SCIENTIFIC
AND CULTURAL
ORGANIZATION

1990 MIRAMARE - TRIESTE

IC/90/381

International Atomic Energy Agency
and
United Nations Educational Scientific and Cultural Organization
INTERNATIONAL CENTRE FOR THEORETICAL PHYSICS

ON THE POSSIBILITY OF LOCALIZING OF ELECTRON GROUP FUNCTIONS USING THE NOTION OF ANTISYMMETRICAL ORTHOGONALITY

Vladimir E. Puchin * and Boris P. Zapol *
International Centre for Theoretical Physics, Trieste, Italy.

MIRAMARE – TRIESTE
November 1990

1. Introduction

The electron group functions (GF) method (see, for example, /1-9/) is recognized as one of the most practically useful and physically transparent methods for the calculation of electronic structure of atoms, molecules, and condensed matter, taking into account the most significant part of electronic correlation. In this approach the many-electron system under consideration is conventionally partitioned into m subsystems, the so-called electron groups (EG), of $N_1, N_2, \ldots, N_m$ electrons ($\sum_{I=1}^{m} N_I = N$). Each of EG's is described by its GF $\Phi_J(X_J)$. Here J is the EG number, X_J is the set of all electron coordinates related to this EG: $X_J = (x_{M_J+1}, \ldots, x_{M_J+N_J})$, where N_J is the number of electrons in J-th EG; $M_J = \sum_{I=1}^{J-1} N_I$; $x_i = (\vec{r}_i, \sigma_i)$ denotes spatial and spin coordinates of i-th electron. GF is usualy supposed to be antisymmetrical with respect to transpositions of its arguments. The wave function of the whole N electron system is constructed as the antisymmetrized product of all the GF's:

$$\Psi(x_1, x_2, \ldots, x_N) = \hat{A} \prod_{J=1}^{m} \Phi_J(X_J), \tag{1.1}$$

where A is an operator performing the antisymmetrization and subsequent normalization of an operand. The GF method in its most consequent form /9-10/ is based on the three following statements.

I. Account for intragroup correlation and complete neglect of intergroup one.

II. Spatial localization of GF's.

III. Variational freedom of the function given in the form (1.1).

Usually all these aspects of the GF method are treated separately. In the present work we should try to consider them jointly seeking to answer the following question. If all these three requirements are

---

* Permanent address: Latvia University, Rainis boul. 19, Riga, 226098 Latvia, USSR.

fulfilled simultaneously, is it the result of a physically adequate choice of partition of N-electron system into N_1, N_2, ...-electron groups? Or, the partition being given, the mathematical techniques of the theory can adapt to these requirements?

More specifically, we try to solve the following problem. Provided that variational freedom is not restricted and intragroup correlation is taken into account in a given approximation, is it possible to develop for GF's any analogue of the well-known (in the case of orbitals) Adams-Gilbert-Kunz method /14-17/ that could give one a possibility to go from delocalized GF's to localized ones seeking for minimization of the intergroup correlation?

2. The physical problem statement

Let us discuss some substantial features of statements I-III paying special attention to their compatibility. The method deals with EG's as entities. The *intragroup* correlation (between the electrons of the same EG) is supposed to be taken into account by any known way. According to the chosen approach the extent of its account can vary from zero (when Φ_J is merely determinant of N_J orbitals while Ψ is that of N ones) till, in principle, complete (when Φ_J is presented, e.g., as infinite series of N_J-th order determinants built on the full basis of orbitals).

On the other hand, if one presents the wave function of the whole system as Eq.(1.1) one introduces immediately the approximation of the complete neglect of *intergroup* correlation. This approach can be treated as development of one-determinantal Hartree-Fock method (where GF's are reduced to orbitals and electronic correlation is completely omitted) for partial account of correlation.

The energy functional $E[\Psi] = \langle\Psi|H|\Psi\rangle$ is minimized over variations of all GF's each being given the *complete variational freedom* restricted only by the normalization constraint. This condition is in fact necessary for the correct account of *intragroup* correlation in *ab-initio* calculations. Imposing additional constraints on GF's leads to the contraction of the class of trial functions and is equivalent to an indirect (and as a result more then likely indefinite) limitation on the extent of account of correlation. Sometimes it can reduce the considered part of intragroup correlation to zero. This statement is corroborated by the practice of the electronic correlation calculations for many-electron systems. It has been observed /11/ that a more complete account of correlation asks the correct choice of basis for the construction of correlated wave functions, the condition corresponding to the requirement of sufficient variational freedom.

Futhermore, GF's are considered to be *localized* in *different* regions of space, so that their spatial overlap is small. This condition, first, provides that *intergroup* correlation effects are small. This may be immediately proved in terms of the density functional method: by virtue of non-linearity of exchange-correlation energy functional the intergroup correlation energy

$$E_{IJ} = E_{xc}[\rho_{IJ}] - E_{xc}[\rho_I] - E_{xc}[\rho_J]$$

is small only if the total electron density $\rho_{IJ}(x)$ is near to either ρ_I or ρ_J in the corresponding regions of space. Second, the localization gives one a basis for a chemical interpretation in terms of transferability of localized GF's. Third, it provides some convenience for numerical realization of the method for extended systems as each GF needs only a basis of functions confined in the corresponding region of space. A substantial simplification of mathematical apparatus of GF method is achieved by imposing the strong orthogonality constraint /5,8,12/ on GF's

$$\int \Phi_I(x,X)\,\Phi_K(x,X')\,dx = 0, \qquad (2.1)$$

X being all arguments of Φ but x. Unfortunately this condition restricts the class of trial functions and worsen their localization. For this reason the method of non-orthogonal GF's is also developed /13,14/.

At first glance the requirements of variational freedom and localization are inconsistent with one another because the latter restricts the former. But not always it is the case. Consider one-determinantal Hartree-Fock method, with

$$\Psi = \hat{A}\left(\varphi_1 \ldots \varphi_N\right). \tag{2.2}$$

Here $\varphi_k(x)$ are one-electron wave functions (for convenience in this work they will be referred to as orbitals) which may be found as decisions of Hartree-Fock equations /12/

$$\hat{F}\,\varphi_i(x) = \varepsilon_i\,\varphi_i(x). \tag{2.3}$$

The important fact is that the same Ψ may be presented also through another set of orbitals, ψ_k's, as

$$\Psi = \hat{A}\left(\psi_1 \ldots \psi_N\right),$$

$\psi_k(x)$ being the decisions of Adams - Gilbert - Kunz equations /15-18/

$$\left(\hat{F} + \hat{\rho}\,\hat{B}\,\hat{\rho}\right)\psi_i(x) = \varepsilon_i'\,\psi_i(x), \tag{2.4}$$

where $\hat{\rho}$ is the operator of one-electron reduced density matrix (RDM-1) of the system, and $\hat{B}$ is an arbitrary hermitian operator. In different applications ψ_k's may be considered as either localized or pseudo-orbitals. Both systems of all { φ_k } and { ψ_k } span the same Hartree-Fock space of decisions of Eq. (2.3). The transition from { φ_i } to { ψ_k } may be performed by a linear transformation

$$\psi_k(x) = \sum_i b_{ik}\,\varphi_i(x), \tag{2.5}$$

Ψ being unchanged as it follows from the properties of determinants. The transformation (2.5) may be used to go from delocalized (φ_k) to localized (ψ_k) orbitals (in fact the degree of maximal possible both localization and delocalization of decisions is restricted by properties of a specific system /19/). Eqs. (2.4) and (2.5) form the basis of a consequent approach to the localized orbitals method /1/.

The set { ψ_k } as well as { φ_k } has the property of complete variational freedom but may be localized. Hence, if correlation is ignored the localisation condition does not restrict the variational freedom. The problem is whether the same can be achieved taking the intragroup correlation into account. In other words, we want to find such a transformation of GF's with arbitrary numbers of electrons which does not change the wave function (1.1) of the whole system with the assumed partition of N electrons into EG's but makes the localization of the GF's possible, similarly to Eqs.(2.5) for orbitals.

If this transformation exists the GF's localization would be achievable without restriction of variational freedom. The localized GF's would satisfy certain "generalized Adams-Gilbert-Kunz" equations, and the GF's method could be considered as free of inherent contradictions. Otherwise one would infer that there is a unique set of GF's which gives a decision of a particular variational problem, the extent of those localization being fixed. As in the final analysis the decision depends on the partition of N electrons into groups and on the way of taking into account the intragroup correlation we may briefly define this case by the formulation "the correlation controls localization". If in the case on hand the GF's turn to be localized it must be considered as a physical effect not a result of choice of a suitable mathematical tool.

3. The antisymmetrical orthogonality of many-electron wave functions

Let us now give the mathematical formulation of the problem. While performing the transformation (2.5) over orbitals one actually adds a zero expression of the form

$$\hat{A}\left[\varphi_i(x_1)\varphi_i(x_2)\varphi_j(x_3)\dots\right]=0 \qquad (3.1)$$

to the N-electron determinantal wave function. As for odd M the equality

$$\hat{A}\left[\Phi_I(x_1\dots x_M)\Phi_I(x_{M+1}\dots x_{2M})\,\Phi_J(x_{2M+1}\dots x_{3M})\right]=0 \qquad (3.2)$$

is valid we conclude that for GF's with the same odd number of electrons, M, the linear transformation

$$\Psi_I(x_1,\dots,x_M)=\sum_J c_{IJ}\,\Phi_J(x_1,\dots,x_M) \qquad (3.3)$$

in the similar manner modifies GF's (and can localize them) but leaves the wave function (1.1) of the system unchanged. One can also easily see that in the general case at even M the equation (3.2) is violated. Hence, Eq. (3.3) gives no decision of the problem at even M. But we can try to obtain the decision in another form.

Let us define the notion of antisymmetrical orthogonality. If two many-electron functions satisfy the equation

$$\hat{A}_{L+M}\left[\Phi(x_1,\dots,x_L)\,\tilde{\Phi}(x_{L+1},\dots,x_{M+L})\right]=0 \qquad (3.4)$$

let us call them mutually antisymmetrically orthogonal (ASO). Here the operator performs the complete antisymmetrization of an operand with respect to all L+M variables, and the numbers of electrons in the two functions, L and M, may differ from one another.

The function (1.1) obviously will not change if we modify any $\Phi_J(x_1,\dots,x_{N_J})$ adding the expression

$$\tilde{\Phi}_I(x_1,\dots,x_{\tilde{N}_I})\;C\,(x_{\tilde{N}_I+1},\dots,x_{N_J}) \qquad (3.5)$$

where $\tilde{\Phi}_I$ is a GF ASO to another GF, Φ_I . Here $\tilde{N}_I \leqslant N_J$, and $C(\dots)$ is an arbitrary coefficient depending on variables $\tilde{\Phi}_I$ "lacks".

It is interesting to find that two functions cannot be strong orthogonal if they are ASO. To show this one has merely to multiply Eq. (3.4) by $\Phi^*(x_1,\dots,x_L)$ and then to integrate over $x_1,\dots,x_L$.

Some examples of ASO functions are given by Eq. (3.2). Let us now present some more examples (see Table 1) to visualize the notion of antisymmetrical orthogonality. We denote 1,2, and 3-particle GF's (orbitals,geminals and trials) by symbols φ , g , and t, and their arguments x_i by i . If arguments are omitted their order is assumed to be natural. a,b,c,... symbolize orthonormal orbitals, α , β , γ , ... are given constants, and C_i are arbitrary constants or functions of necessary arguments. r is the rank of the corresponding RDM-1. Each of $\tilde{\Phi}$ in the Table 1 is ASO to the corresponding Φ as may be immediately checked by substituting them into Eq. (3.4). Moreover, if one has $\tilde{\Phi}_M$ ASO to a given Φ_L then it is always possible to construct $\tilde{\Phi}_{M'}$ with M'>M, also ASO to Φ_L , making mere replacement of C_i's by arbitrary functions of "lacked" arguments built on non-occupied natural orbitals.

The following part of the paper deals with the investigation of necessary and sufficient conditions of the existence of functions ASO to a given one.

Table 1

L	r	$\phi(1,\ldots,L)$	M	$\tilde\phi(1,\ldots,M)$
1	1	$\varphi(1)$	1 2	$\tilde\varphi(1) = \varphi(1)$ $\tilde g(1,2) = \hat A\, C_1(1)\varphi(2)$
2	2	$g(1,2) = \hat A\, a(1)b(2)$	1 2	$\tilde\varphi(1) = 0$ $\tilde g(1,2) = C_1\, g(1,2) +$ $+\hat A[C_2(1)a(2) + C_3(1)b_2(2)]$
2	4	$g(1,2) = \hat A[\alpha a(1)b(2) +$ $+\beta c(1)d(2)]$	1 2	$\tilde\varphi(1) = 0$ $\tilde g = \hat A[C_1 ac + C_2 ad + C_3 bc +$ $+C_4 bd + C_5(\beta ab - \alpha cd)]$
2	6	$g(1,2) = \hat A[\alpha ab +$ $+\beta cd + \gamma ef]$	1 2 3	$\tilde\varphi = 0$ $\tilde g = 0$ $\tilde t = \hat A[C_1 ace + C_2 acf +$ $+C_3 bce + C_4 bcf + C_5 ade +$ $+C_6 adf + C_7 bde + C_8 bdf +$ $+(C_9 a + C_{10} b)(\gamma cd - \beta ef) +$ $+(C_{11} c + C_{12} d)(\gamma ab - \alpha ef) +$ $+(C_{13} e + C_{14} f)(\beta ab - \alpha cd)]$
3	6	$t = \hat A(\alpha abc + \beta ade +$ $+\gamma bdf + \delta cef)$	1 2	$\tilde\varphi = 0$ $\tilde g = \hat A[C_1 af + C_2 be + C_3 cd +$ $+C_4(\alpha ef - \delta ab) + C_5(\gamma ae -$ $-\beta bf) + C_6(\beta bc - \alpha de) +$ $+C_7(\gamma ac - \alpha df) + C_8(\beta cf -$ $-\delta ad) + C_9(\delta cd - \beta bd)]$

4. Conditions of existence of ASO geminals

We begin with the simple case L=M=2. Let geminal g(1,2) be given. We have to solve the equation

$$\hat A\ (1234)\ g(1,2)\,\tilde g(3,4) = 0, \qquad (4.1)$$

where $\tilde g$ is the unknown function. Both g and $\tilde g$ are supposed to be antisymmetrical:

$$\hat A(1,2)\ g(1,2) = g(1,2);$$
$$\hat A(12)\ \tilde g(1,2) = \tilde g(1,2). \qquad (4.2)$$

Let us denote natural orbitals of g as φ_k. Then we can write /12/

$$g(1,2) = \sum_{ik} c_{ik}\ \varphi_i(1)\,\varphi_k(2). \qquad (4.3)$$

It follows from (4.2) that

$$c_{ik} = -c_{ki}\ ;\quad c_{kk} = 0. \qquad (4.4)$$

Let us substitute (4.3) and (4.5) into (4.1). Making use of the right coset decomposition of symmetrical group S_4 with respect to its subgroup $S_2 \otimes S_2$ which generates the corresponding decomposition of the antisymmetrizer /13, 14/

$$\hat A\ (1234) = \hat A^R \hat A\,(12)\,\hat A(34) \qquad (4.6)$$

with

$$\hat A^R = \frac{1}{6}\left\{\hat E - \hat P_{13} - \hat P_{14} - \hat P_{23} - \hat P_{24} + \hat P_{12}\hat P_{34}\right\}, \qquad (4.7)$$

where $\hat P_{ij}$ is the permutation of arguments i and j and $\hat E$ is identity permutation, and taking into account Eq.(4.2) we obtain

$$\sum_{iklm} c_{ik} a_{lm} \{ \varphi_i \varphi_k \varphi_l \varphi_m - \varphi_l \varphi_k \varphi_i \varphi_m - \varphi_i \varphi_l \varphi_k \varphi_m - \varphi_m \varphi_k \varphi_l \varphi_i - \varphi_i \varphi_m \varphi_l \varphi_k + \varphi_l \varphi_m \varphi_i \varphi_k \} = 0 \tag{4.8}$$

where the first function in each term has the argument x_1, the second x_2 and so on. As a summation with respect to each of the indices i, k, l, and m extends over all set we may re-label them to obtain

$$\sum_{iklm} \varphi_i(1)\varphi_k(2)\varphi_l(3)\varphi_m(4) \{ c_{ik} a_{lm} - c_{lk} a_{im} - c_{il} a_{km} - c_{mk} a_{li} - c_{im} a_{lk} + c_{lm} a_{ik} \} = 0. \tag{4.9}$$

The mutual linear independence of the functions φ_i yields then the following system of equations for unknown coefficients a_{ln}:

$$c_{ik} a_{lm} - c_{lk} a_{im} - c_{il} a_{km} - c_{mk} a_{li} - c_{im} a_{lk} + c_{lm} a_{ik} = 0, \tag{4.10}$$

which may be presented in a more compact form as

$$\hat{A}^R (iklm)\ c_{ik} a_{lm} = 0. \tag{4.11}$$

The operator A here is assumed to antisymmetrize its operand with respect to permutations of 4 indices taking into account the properties (4.3) and (4.5) in the way similar to that used in Eq.(4.6). Eqs.(4.10) present the basic equations to define ASO geminals. The system is linear and homogeneous, and the known values $\{c_{ik}\}$ are its coefficients.

Now let us distinguish occupied and unoccupied natural orbitals. If

$$c_{in} = 0 \tag{4.13}$$

for all i and a given n then the n-th natural orbital is called unoccupied. The occupation number ν_k (i.e. the k-th eigenvalue of RDM-1) satisfies the formula /20/

$$\sum_l c_{kl} c^*_{ml} = \nu_k \delta_{km}. \tag{4.14}$$

For unoccupied natural orbitals

$$\nu_n = 0. \tag{4.15}$$

Let us denote r the number of occupied states (it is the rank of RDM-1). Sums in Eqs.(4.3) and (4.14) actually are taken over the occupied states only ("Fermi sea").

Consider Eqs.(4.10) for the case when states i,k are occupied, but l,m are not. Accounting for (4.13) one obtains

$$a_{lm} = 0, \qquad l, m \ \text{unoccupied}. \tag{4.16}$$

If i,k,l are occupied states, but m is not, Eqs.(4.10) take the form

$$c_{ik} a_{lm} + c_{kl} a_{im} + c_{li} a_{km} = 0. \tag{4.17}$$

The system (4.10) obviously breaks up to subsystems each corresponding to its own unoccupied m. For a given m, all i,k,l values differ from one another by virtue of (4.4). For each m the system (4.17) contains r unknowns and $\binom{r}{3}$ equations. Hence, for r<4 we have less equations than unknowns, and there is infinite number of $\tilde{g}$'s built on occupied and/or unoccupied natural orbitals in compliance with Eqs.(4.17). If r = 4 we have r both unknowns and equations. The equations would have nontrivial decision at zero system determinant.But for r=4 this determinant is nonzero due to the positive definiteness of RDM-1. Hence, the system (4.17) has no decision for $r \geqslant 4$.

Now let all indices i,k,l,m correspond to occupied states. Then there is $\binom{r}{2}$ unknown values a_{ik} and $\binom{r}{4}$ equations (4.17) for them. While r < 6 the number of equations exceeds the number of unknowns, and the decision may occur. For r $\geqslant 6$ there is no decision.

So if the rank of a given geminal is less than 6 it has non-trivial ASO geminals (cf. Table 1).

5. Conditions of antisymmetrical orthogonality in the common case

The generalization of the consideration given in the previous section to the common case of antisymmetrical orthogonality between a given L-electron function $\Phi(L)$ and unknown M-electron function $\tilde{\Phi}(M)$ is straightforward. Expanding both functions in terms of natural orbitals of $\Phi(L)$,

$$\Phi(1,\dots,L)=\sum_{i_1\dots i_L} C_{i_1\dots i_L}\varphi_{i_1}(1)\dots\varphi_{i_L}(L), \tag{5.1}$$

$$\tilde{\Phi}(1,\dots,M)=\sum_{k_1\dots k_M} C_{k_1\dots k_M}\varphi_{k_1}(1)\dots\varphi_{k_M}(M), \tag{5.2}$$

then substituting both expansions in the equation (3.4), and then making use of linear independence of natural orbitals $\{\varphi_i\}$, we obtain the system of equations

$$\hat{A}^{R}_{L+M}\, C_{i_1\dots i_L}\, a_{i_{L+1}\dots i_{L+M}}=0. \tag{5.3}$$

Let r again be the rank of RDM-1. Consider the system for the case when s of all L+M indices i_K correspond to occupied states while remaining L+M−s to unoccupied ones. s is restricted by the condition

$$L\leq s\leq \min(r, L+M). \tag{5.4}$$

The system (5.3) again splits to unconnected subsystems each for its own complect of unoccupied indices. Let these indices be fixed while other s run over all occupied states remaining mutually different. Then $a_{i_1\dots i_M}$ has M−(L+M−s) = s−L indices labelling occupied states. It gives $\binom{r}{s-L}$ unknowns. The number of equations is $\binom{r}{s}$, and the condition of existence of nontrivial solution for the chosen part of system (5.3) reads as

$$\binom{r}{s}<\binom{r}{s-L}. \tag{5.5}$$

It is equivalent to

$$\left|\frac{r}{2}-s\right|<\left|\frac{r}{2}-s+L\right|. \tag{5.6}$$

If both inequalities (5.4) and (5.6) are satisfied, at least at one s value, one may conclude that $\tilde{\Phi}(M)$ ASO to a given $\Phi(L)$ of rank r exists. The simultaneous investigation of unequalities (5.4) and (5.6) shows that it takes place if

$$2M\geqslant r+1-L. \tag{5.8}$$

6. Discussion and summary

As it follows from Eq.(5.8), the improvement of quality of account of correlation in the function $\Phi(L)$ that is raising of a difference r-L causes the increase of the minimal M value necessary for existance of a $\tilde{\Phi}(M)$ ASO to $\Phi(L)$. This fact restricts the possibilities of simultaneous localization of GF's and account for their intragroup correlation, especialy for small L values. But the restriction becomes less severe when L rises. Let us consider valence shells of anions in alcali halide crystal as an example of GF's. Then L=M=8, so that GF rank is constraint by inequality r<24. It means, that up to 15 excited natural orbitals may be used, which gives 490314 determinants in a CI expansion of GF.

So we see that in some cases a compromise may be achieved between the assumptions I, II, and III of the GF theory. We can conclude that the notion of antisymmetrical orthogonality of many-electron functions introduced in the present paper presents an additional theoretical foundation of the GF method and gives one a possibility of a more in-depth study of the substantial assumptions of this approach and, in some cases, also improvement of its power.

ACKNOWLEDGMENTS

The authors would like to thank Professor Abdus Salam, the International Atomic Energy Agency and UNESCO for hospitality at the International Centre for Theoretical Physics, Trieste, where this work was done.

REFERENCES

1.A.M.Stoneham,Theory of Defects in Solids (Clarendon,Oxford, 1975)
2.L.Szasz,Z.Naturforschung 14a, 1014 (1959)
3.R.K.Nesbet,Adv.Chem.Phys.14,1 (1969)
4.K.B.Tolpygo,Usp.Fiz.Nauk 74, 269 (1971)
5.I.Lyast,Zh.Strukt.Khimii 16, 379 (1975)
6.I.Lyast,Phys.Mol.(Soviet)2, 41, (1976)
7.V.A.Telezhkin,K.B.Tolpygo,Fiz.Tekhn.Poluprov.16, 1337 (1982)
8.S.Wilson,Electron correlations in molecules(Clarendon,Oxford,1984)
9.L.Kantorovich and references therein
10.W.J.Hunt, P.J.Hay, W.A.Goddard III, J.Chem.Phys. 57, 738 (1972)
11.Correlation Effects in Atoms and Molecules. Eds:R.Lefebvre and C.Moser (Interscience,London et al, 1969)
12.R.McWeeny and B.T.Sutcliffe, Methods of Molecular Quantum Mechanics (Academic, London,1969)
13.L.Kantorovich,B.Zapol, J.Chem.Phys.(submitted)
14.D.J.Klein. In: Group Theory and its Applications,Vol.3. Ed.:M.Loebl (Academic,N.-Y.,1965), p.1-93.
15.W.H.Adams,J.Chem.Phys.34,89(1961)
16.T.L.Gilbert, . In: Molecular Orbitals in Chemistry,Physics and Biology. Ed.: P.O.Lowdin (Academic, N.-Y.,1964)
17.A.B.Kunz,Phys.status solidi 36,301 (1969)
18.A.B.Kunz Phys Rev. B26, 2056 (1982)
19.J.Pipek, Int.J.Quant.Chem. 36, 487 (1989)
20.A.J.Coleman, Adv.Mod.Phys.35, 668 (1963)

Stampato in proprio nella tipografia
del Centro Internazionale di Fisica Teorica