THEORETICA CHIMICA ACTA

Theoret. Chim. Acta (Berl.) 61, 135–147 (1982)

Orbital Forms of Gap Equations and Instability Conditions

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Previously derived forms of instability conditions at the spin orbital level are specialized to orbital levels of different kinds. Similarly the special forms of the gap equation that are obtained for different types of broken symmetry solutions are analyzed and discussed.

Key words: Gap equation – Instabilities – Fukutome classes.

1. Introduction

Correlation in electronic systems is usually associated with "anything going beyond Hartree–Fock". The term "Hartree–Fock" then normally means restricted Hartree–Fock (RHF) and the most common restriction is that two electrons with different spins are associated with the same orbital. The term unrestricted Hartree–Fock (UHF) is often used for a situation where that particular restriction of doubly filled orbitals is removed. There are also other restrictions however. Even in UHF the spin orbitals are normally simple products of an orbital and a spin function, and in practice the orbitals are often restricted to be real functions.

A method in which the total wave function is approximated by a single determinant built up of general spin orbitals (GSO),

$$\psi_k(x) = \phi_{k1}(\boldsymbol{r})\alpha(\zeta) + \phi_{k2}(\boldsymbol{r})\beta(\zeta),$$

where the orbital components ϕ_{k1} and ϕ_{k2} can be complex, might be called the general Hartree–Fock method (GHF). In contrast to the symmetry restricted RHF spin orbitals those occurring in the GHF (UHF) procedure are of so-called broken symmetry type. That expression does not imply, however, that they have

* Supported by the Swedish Natural Sciences Research Council.

0040-5744/82/0061/0135/$02.60

no symmetry at all. Even in such cases the effective one electron operator usually commutes with certain symmetry operations and the spin orbitals transform according to one of the irreducible representation or co-representations of the corresponding group. That group is then a subgroup of the full group of the basic many electron Hamiltonian, and the GHF spin orbitals in general have a lower symmetry than the RHF spin orbitals.

A systematic way of classifying different types of GHF solutions has been developed by Fukutome [1]. Irrespective of any spatial symmetries the total Hamiltonian commutes with all spin rotations and time reversal. If the effective one electron Hamiltonian $\mathscr{H}_{\text{eff}}$, also commutes with all these operations we have the RHF case. If on the other hand $\mathscr{H}_{\text{eff}}$ only commutes with the elements of a subgroup, we have one of the broken symmetry cases. Including the trivial subgroups there are eight such inequivalent subgroups and every GHF solution must therefore "belong" to one of the corresponding eight classes.

The association of a GHF solution to such a class means therefore that the corresponding spin orbitals transform according to the irreducible representations or co-representations of the subgroup in question. The properties of such a set of spin orbitals are best described with reference to their Fock–Dirac matrix. The orbital components of that matrix—the number density matrix and the spin density vector—can be real or complex. The spin density matrix vector can have one or more vanishing components, and its direction can be fixed in space or vary with position.

An extension of this scheme to include also spatial point group symmetry has been developed by Ozaki and Fukutome [2]. An algorithm for obtaining all double valued irreducible (co-) representations for the corresponding groups has been constructed by Ozaki [3].

The transition from a class of GHF solutions characterized by a certain subgroup to one with a smaller group is associated with an instability. From the point of view of the variational principle this means that the extremum obtained with spin orbitals of the higher symmetry is unstable with respect to variations leading to the particular kind of lower symmetry. Thouless [4] seems to have been the first one to formulate explicit stability conditions for Hartree–Fock functions. In quantum chemistry the names Cizek–Paldus [5] and Fukutome [6] mark important developments in this area. A slightly different formulation of the problem has been given recently [7]; in this paper we also give a relatively extensive list of papers in this field by the previously mentioned authors and their collaborators. The conditions for instability are associated with the appearance of negative eigenvalues of a certain matrix, and the corresponding eigenvectors give information as to where in function space one should look for the broken symmetry solutions.

In order to find explicit broken symmetry solutions we have to go beyond the instability conditions, however. An interesting procedure for doing that, which has proved powerful in many applications, is by means of so-called pairing [8].

Each spin orbital of higher symmetry (normally the RHF spin orbitals) is paired with a spin orbital from the orthogonal complement of the occupied higher symmetry spin orbitals. This procedure constitutes a natural extension of the way the instability conditions are formulated in Ref. 7. The strength of this pairing is determined by the variational principle, and the resulting conditions can be formulated as an integral equation for a "gap function" – the gap equation [8], [9]. The gap equation has been solved explicitly for a few model systems [10]–[13]. The results are encouraging and there are reasons to believe that this method will provide an efficient and explicit way of taking at least certain kinds of correlation in large systems into account.

Both the instability conditions and the gap equation are primarily formulated at a general spin orbital level. Fukutome's classification makes it possible to distinguish eight different cases. A derivation of the form of the corresponding pairs of spin orbitals has recently been given [14]. In order to proceed further we need to go from the spin orbital to the orbital level. This will mean a specialization of the concepts of singlet and non-singlet instability [5]–[7].

The purpose of the present paper is to derive orbital forms of instability conditions and gap equations. We will do this in a few typical cases which can be expected to be the most useful ones. At the same time this will illustrate the general method which can be applied in other cases as well.

2. Orbital Forms of Instability Conditions

Our starting point is the formulation of the stability problem presented in Ref. 7. A variationally defined extremum with a single determinant total wave function is unstable if the matrix

$$\mathfrak{T} = \begin{bmatrix} \mathfrak{A}_1 + \mathfrak{B}_1 & -\mathfrak{A}_2 + \mathfrak{B}_2 \\ \mathfrak{A}_2 + \mathfrak{B}_2 & \mathfrak{A}_1 - \mathfrak{B}_1 \end{bmatrix}, \tag{1}$$

has at least one negative eigenvalue. The size of this matrix is $(2N)\times(2N)$, where N is the number of electrons in the system considered. The $N \times N$ matrices $\mathfrak{A}_i$ and $\mathfrak{B}_i$ are real. $\mathfrak{A}_1$ and $\mathfrak{B}_1$ are the real and $\mathfrak{A}_2$, $\mathfrak{B}_2$ the imaginary parts of the matrices

$$\mathfrak{A} = \mathfrak{A}_1 + i\mathfrak{A}_2; \qquad \mathfrak{B} = \mathfrak{B}_1 + i\mathfrak{B}_2, \tag{2}$$

defined by

$$\begin{aligned} A_{kl} &= \langle D_k | Q | D_l \rangle; \\ B_{kl} &= \langle D_{kl} | Q | D \rangle. \end{aligned} \tag{3}$$

Here D is the reference determinant associated with the extremum point that is investigated, and D_k, D_{kl} denote determinants which are singly and doubly "excited" with respect to this reference determinant, respectively. The operator Q is

$$Q = \mathscr{H} - E \cdot 1, \tag{4}$$

where $\mathcal{H}$ is the total Hamiltonian of the system and E its expectation value with respect to D. Explicit expressions for the matrix elements of $\mathfrak{A}$ and $\mathfrak{B}$ in terms of the spin orbitals used are given in Ref. 7.

For spin orbitals we use a spinor notation,

$$\begin{aligned}\psi_k(x) &= \phi_{k1}(\boldsymbol{r})\alpha(\zeta) + \phi_{k2}(\boldsymbol{r})\beta(\zeta) \\ &= (\alpha, \beta)\begin{pmatrix}\phi_{k1}\\ \phi_{k2}\end{pmatrix} = (\alpha, \beta)\boldsymbol{\Phi}_k,\end{aligned} \tag{5}$$

and we will normally write out only the orbital components Φ_k. These are in general complex. Similarly we will work with the orbital form $\mathfrak{Q}$ of the Fock–Dirac density matrix,

$$\boldsymbol{\rho} = |\psi\rangle\langle\psi| = (\alpha\beta)\mathfrak{Q}\begin{pmatrix}\alpha\\ \beta\end{pmatrix}. \tag{6}$$

The 2×2 matrix $\mathfrak{Q}$ can be expressed in terms of the number density matrix N and the spin density matrix vector $\boldsymbol{S}$,

$$\mathfrak{Q} = \tfrac{1}{2}N\cdot\mathbf{1} + \boldsymbol{\sigma}\cdot\boldsymbol{S} \tag{7}$$

The vector $\boldsymbol{\sigma}$ has the Pauli matrices as components.

The fundamental quantity for stability analyses is the second variation, $\delta^2 E$, of the total energy, that is obtained when the spin orbitals ψ_k of the reference determinant D are replaced by

$$\phi'_k = \frac{1}{\sqrt{1+|c_k|^2}}(\psi_k + c_k\bar{\psi}_k). \tag{8}$$

Here $\bar{\psi}_k$ is a function in the orthogonal complement of the set $\{\psi_k\}$ that is used in D and c_k is an arbitrary complex number. In order to connect different but related notations we give three forms of $\delta^2 E$ [7],

$$\begin{aligned}\delta^2 E &= \mathfrak{d}^+\mathfrak{T}\mathfrak{d} \\ &= \sum_{k,l=1}^{N}\{c_k^* A_{kl}c_l + \tfrac{1}{2}[c_k^* B_{kl}c_l^* + c_k B_{kl}^* C_l]\} \\ &= \int [F(1)\delta^2 N(1,1') + 2\boldsymbol{G}(1)\cdot\delta^2\boldsymbol{S}(1,1')]\,dv_1 \\ &\quad + \frac{1}{2}\int\frac{\delta N(1,1)\delta N(2,2)}{r_{12}}\,dv_1\,dv_2 - \frac{1}{4}\int\frac{\delta N(1,2)\delta N(2,1)}{r_{12}}\,dv_1\,dv_2 \\ &\quad - \int\frac{\delta\boldsymbol{S}(1,2)\cdot\delta\boldsymbol{S}(2,1)}{r_{12}}\,dv_1\,dv_2.\end{aligned} \tag{9}$$

Here d_k are the real and imaginary components of $c_k = a_k + ib_k$, obtained by doubling the size of the column vector $\mathfrak{c}$:

$$\mathfrak{c} = \mathfrak{a} + i\mathfrak{b}; \qquad \mathfrak{d} = \begin{bmatrix} \mathfrak{a} \\ \mathfrak{b} \end{bmatrix}. \tag{10}$$

The operators $F(1)$ and $\boldsymbol{G}(1)$ are the orbital forms of the effective one electron Hartree–Fock operator associated with the reference determinant D,

$$F(1) = h_1 + \int dv_2 \frac{N(2,2)}{r_{12}} - \frac{1}{2}\int dv_2 \frac{P^r_{12}N(2,2')}{r_{12}},$$

$$\boldsymbol{G}(1) = -\int dv_2 \frac{P^r_{12}\boldsymbol{S}(2,2')}{r_{12}} \tag{11}$$

The arguments of N and $\boldsymbol{S}$ in (10) and (11) have been abbreviated so that 1 stands for $\boldsymbol{r}_1$, etc.

Then we need the general form of the spin orbitals in the eight Fukutome classes. We sum up what has been obtained elsewhere [1], [14] by showing for each class the set of occupied spinors. We thus write

$$|\psi\rangle = [\psi_1, \psi_2, \ldots, \psi_N] = (\alpha, \beta)|\Phi\rangle;$$

$$|\Phi\rangle = [\Phi_1, \Phi_2, \ldots \Phi_N] = \begin{bmatrix} \phi_{11}, \phi_{21}, \ldots \phi_{k1}, \ldots \phi_{N1} \\ \phi_{12}, \phi_{22}, \ldots \phi_{k2}, \ldots \phi_{N2} \end{bmatrix}. \tag{12}$$

2.1. *T(ime) (reversal) I(nvariant) C(losed) S(hells)*

$$|\Phi\rangle = \begin{bmatrix} u_1, 0, u_2, 0, \ldots u_{N/2}, 0 \\ 0, u_1, 0, u_2, \ldots 0, u_{N/2} \end{bmatrix}; \tag{13}$$

the orbitals $u_i(\boldsymbol{r})$ are real.

2.2. *C(harge) C(urrent) W(aves)*

Same as for TICS but with complex orbitals $u_i(\boldsymbol{r})$.

2.3. *A(xial) S(pin) C(urrent) W(aves)*

$$|\Phi\rangle = \begin{bmatrix} u_1, 0, u_2, 0, \ldots u_{N/2}, 0, \\ 0, u_1^*, 0, u_2^*, \ldots 0, u_{N/2}^* \end{bmatrix}. \tag{14}$$

2.4. *A(xial) S(pin) D(ensity) W(aves)*

$$|\Phi\rangle = \begin{bmatrix} u_1, 0, u_2, 0, \ldots u_{N/2}, 0 \\ 0, v_1, 0, v_2, \ldots 0, v_{N/2} \end{bmatrix}; \tag{15}$$

the orbitals $u_i(\boldsymbol{r})$ and $v_i(\boldsymbol{r})$ are real.

2.5. A(xial) S(pin) W(aves)

Same as (15) but with complex orbitals u_i and v_i.

2.6. T(orsional) S(pin) C(urrent) W(aves)

$$|\Phi\rangle = \begin{bmatrix} u_1, w_1, u_2, w_2, \ldots u_{N/2}, w_{N/2} \\ -w_1^*, u_1^*, -w_2^*, u_2^*, \ldots -w_{N/2}^*, u_{N/2}^* \end{bmatrix}. \tag{16}$$

2.7. T(orsional) S(pin) D(ensity) W(aves)

$$|\Phi\rangle = \begin{bmatrix} u_1, w_1, u_2, w_2, \ldots u_{N/2}, w_{N/2} \\ t_1, v_1, t_2, v_2, \ldots t_{N/2}, v_{N/2} \end{bmatrix}; \tag{17}$$

the orbitals $u_i(\boldsymbol{r})$, $t_i(\boldsymbol{r})$, $w_i(\boldsymbol{r})$, and $v_i(\boldsymbol{r})$ are real.

2.8. T(orsional) S(pin) W(aves)

Same as (17) but with complex orbitals.

When we know that the spin orbitals in D belong to one of these classes and want to study the possibility of an instability towards another class, it is in most cases possible to simplify the second variation (9) so as to reduce the size of the matrix (1). If we go from TICS to TICS or to ASDW, from ASDW to ASDW or to TSDW, or from TSDW to TSDW, all orbitals remain real. In such a case we have

$$\delta^2 E = \mathfrak{d}^+ \tilde{\mathfrak{T}} \mathfrak{d} = (\tilde{\mathfrak{a}} \mathbf{0}) \tilde{\mathfrak{T}} \begin{pmatrix} \mathfrak{a} \\ \mathbf{0} \end{pmatrix} = \tilde{\mathfrak{a}} (\mathfrak{A}_1 + \mathfrak{B}_1) \mathfrak{a}, \tag{18}$$

and we only have to find the eigenvalues of the $N \times N$ matrix $\mathfrak{A}_1 + \mathfrak{B}_1$. A similar reduction is obtained if we require all spin orbitals ψ_k and $\bar{\psi}_k$ in (8) to be real, but use purely imaginary coefficients c_k. Then

$$\delta^2 E = \mathfrak{d}^+ \tilde{\mathfrak{T}} \mathfrak{d} = (\mathbf{0} \tilde{\mathfrak{b}}) \tilde{\mathfrak{T}} \begin{pmatrix} \mathbf{0} \\ \mathfrak{b} \end{pmatrix} = \tilde{\mathfrak{b}} (\mathfrak{A}_1 - \mathfrak{B}_1) \mathfrak{b}. \tag{19}$$

This type of reduction is obtained when we go from TICS to CCW or ASW to ASDW to ASW or from TSDW to TSW.

This is still at the spin orbital level. To acheive further reductions we go over to the orbital form of the instability conditions in a few illustrative cases. In the formulation of the problem that is used here different cases are obtained from different choices of the varied functions, i.e. the $\bar{\psi}_k$ and their coefficients c_k in (8).

If we start out from a reference determinant with doubly filled orbitals, i.e. of TICS or CCW type, it seems natural to choose the coefficients in pairs such that

$$c_{2k'-1} = c_{2k'} = \bar{c}_{k'}; \qquad k' = 1, 2, \ldots, \frac{N}{2}. \tag{20}$$

Then the second variation can be written

$$\delta^2 E = \sum_{k',l'=1}^{N/2} [\bar{c}^*_{k'} \bar{A}_{k'l'} \bar{c}_{l'} + \tfrac{1}{2}(\bar{c}^*_{k'} \bar{B}_{k'l'} \bar{c}^*_{l'} + \bar{c}_{k'} \bar{B}^*_{k'l'} \bar{c}_{l'})], \tag{21}$$

with

$$\bar{A}_{k'l'} = A_{2k'-1,2l'-1} + A_{2k'-1,2l'} + A_{2k',2l'-1} + A_{2k',2l'}, \tag{22}$$

and $\bar{B}_{k'l'}$ defined in a similar way. We now have to find the eigenvalues of a complex $(N/2)\times(N/2)$ matrix. By means of the procedure used in Ref. 7 that problem can be reformulated in terms of a real N×N matrix

$$\delta^2 E = \bar{\mathfrak{d}}^+ \mathfrak{Z} \bar{\mathfrak{d}}; \tag{23a}$$

$$\bar{\mathfrak{d}} = \begin{pmatrix} \bar{\mathfrak{a}} \\ \bar{\mathfrak{b}} \end{pmatrix}; \qquad \bar{\mathfrak{c}} = \bar{\mathfrak{a}} + i\bar{\mathfrak{b}}; \tag{23b}$$

$$\mathfrak{Z} = \begin{bmatrix} \bar{\mathfrak{A}}_1 + \bar{\mathfrak{B}}_1 & -\bar{\mathfrak{A}}_2 + \bar{\mathfrak{B}}_2 \\ \bar{\mathfrak{A}}_2 + \bar{\mathfrak{B}}_2 & \bar{\mathfrak{A}}_1 - \bar{\mathfrak{B}}_1 \end{bmatrix}. \tag{23c}$$

Cases with real orbitals then reduce to $(N/2)\times(N/2)$ problems like

$$\delta^2 E = \tilde{\bar{\mathfrak{a}}}(\bar{\mathfrak{A}}_1 + \bar{\mathfrak{B}}_1)\bar{\mathfrak{a}}, \tag{24}$$

in analogy to (18), whereas with real orbitals but purely imaginary coefficients $\bar{c}_k$ are reduced like (19):

$$\delta^2 E = \tilde{\bar{\mathfrak{b}}}(\bar{\mathfrak{A}}_1 - \bar{\mathfrak{B}}_1)\bar{\mathfrak{b}}. \tag{25}$$

Particular cases of (23), (24) and (25) are obtained by specifying reference spin orbitals ψ_k and varied spin orbitals ϕ'_k [8] according to (13)–(17). Then the spin integration can be carried out explicitly in the matrix elements A_{kl} and B_{kl}. The result is an orbital form of the instability problem which is valid for the particular pair of classes chosen.

The type of reduction of the instability problem that is illustrated by the choice (20) is just one example. The combination of the formulation of the instability problem used in Ref. 7 and the particular forms of the spin orbitals (13)–(17) leads in each specific case to certain simplifications. Within the resulting form of $\delta^2 E$ obtained in that way we can then exploit the remaining degrees of freedom.

3. Orbital Forms of Gap Equations

We start out from the general derivation of a gap equation given in Ref. 8. For that purpose we modify the notations slightly as compared to those of the previous section.

The basic idea is to construct GHF spin orbitals of a more general kind than those used in RHF, by pairing occupied and virtual RHF spin orbitals:

$$\begin{aligned} &\phi'_\mu = \psi_\mu u_\mu + \bar{\psi}_\mu v_\mu; \\ &u_\mu^2 + v_\mu^2 = 1. \end{aligned} \tag{26}$$

The coefficients u_μ and v_μ are chosen real but the relative phases of ψ_μ and $\bar{\psi}_\mu$ are included in the definition of $\bar{\psi}_\mu$. For a given choice of virtual spin orbitals $\bar{\psi}_\mu$ the strength of the pairing is determined by minimizing the expectation value of the determinant

$$D' = \frac{1}{\sqrt{N!}} \det\{\phi'_\mu\}, \tag{27}$$

with respect to the coefficients u_μ (or v_μ). The N conditions obtained in that way can be combined in an equation for the gap function

$$\Delta_\mu = -\int \mathscr{H}'_{\text{eff}}(1)\sigma_\mu(x_1, x'_1)\, dx_1. \tag{28}$$

Here

$$\sigma_\mu(x, x') = \psi_\mu(x)\bar{\psi}^*_\mu(x') + \bar{\psi}_\mu(x)\psi^*_\mu(x'), \tag{29}$$

and $\mathscr{H}'_{\text{eff}}$ is the effective one electron operator associated with (27)

$$\mathscr{H}'_{\text{eff}}(1) = h_1 + \int dx_2 \frac{(1 - P_{12})\rho'(x_2, x'_2)}{r_{12}}; \tag{30a}$$

$$\rho'(x, x') = \sum_{\mu=1}^{N} \phi'_\mu(x)\phi'^*_\mu(x'). \tag{30b}$$

The extremum conditions can be written as

$$e_\mu = \frac{\lambda_\mu}{\sqrt{1 - \lambda_\mu^2}} \Delta_\mu, \tag{31}$$

where

$$\begin{aligned} e_\mu &= \int \mathscr{H}'_{\text{eff}}(1)\tau_\mu(x_1, x'_1)\, dx_1; \\ \tau_\mu(x, x') &= \bar{\psi}_\mu(x)\bar{\psi}^*_\mu(x') - \psi_\mu(x)\psi^*_\mu(x'), \end{aligned} \tag{32}$$

and

$$\lambda_\mu = u_\mu^2 - v_\mu^2. \tag{33}$$

The gap equation is obtained by combining (28), (29), (30), (31), (32), and (33):

$$\begin{aligned} \Delta_\mu = -\frac{1}{2}\sum_\nu \int dx_1\, dx_2 \frac{(1 - P_{12})\sigma_\mu(x_1, x'_1)}{r_{12}} \\ \times \left\{ \frac{\sigma_\nu(x_2, x'_2)\Delta_\nu}{\sqrt{e_\nu^2 + \Delta_\nu^2}} + \tau_\nu(x_2, x'_2)\left[1 - \frac{e_\nu}{\sqrt{e_\nu^2 + \Delta_\nu^2}}\right] \right\}. \end{aligned} \tag{34}$$

Since the quantities e_ν, (32), can be written in a form similar to (34) we have in general two coupled equations for Δ and e. We can normally expect ψ_μ to be

a more important component in ϕ'_μ than $\bar{\psi}_\mu$. Writing

$$u_\mu = \cos\theta_\mu; \qquad v_\mu = \sin\theta_\mu, \tag{35}$$

we therefore choose

$$0 \leq \theta_\mu \leq \frac{\pi}{4}, \tag{36}$$

so that

$$\begin{aligned} &\frac{1}{\sqrt{2}} \leq u_\mu \leq 1; \\ &0 \leq v_\mu \leq \frac{1}{\sqrt{2}}. \end{aligned} \tag{37}$$

The quantities e_μ and Δ_μ then have the same sign and we have

$$0 \leq \frac{\Delta_\mu}{e_\mu} < \infty. \tag{38}$$

We introduce the notations

$$\begin{aligned} J_{\mu\nu} &= \int dx_1\, dx_2 \frac{1}{r_{12}} (1 - P_{12}) \sigma_\mu(x_1, x'_1) \sigma_\nu(x_2, x'_2); \\ K_{\mu\nu} &= \int dx_1\, dx_2 \frac{1}{r_{12}} (1 - P_{12}) \sigma_\mu(x_1, x'_1) \tau_\nu(x_2, x'_2), \end{aligned} \tag{39}$$

so that the gap Eq. (34) can be written

$$\Delta_\mu = -\frac{1}{2} \sum_\nu \left\{ \frac{J_{\mu\nu} \Delta_\nu}{\sqrt{e_\nu^2 + \Delta_\nu^2}} + K_{\mu\nu} \left[1 - \frac{e_\nu}{\sqrt{e_\nu^2 + \Delta_\nu^2}} \right] \right\}. \tag{40}$$

We further notice that the general orbital forms of the quantities Δ_μ and e_μ are

$$\Delta_\mu = -\int \bar{\mathbf{\Phi}}^+_\mu(1) \mathfrak{H}'(1) \mathbf{\Phi}_\mu(1)\, dv_1 - \int \mathbf{\Phi}^+_\mu(1) \mathfrak{H}'(1) \bar{\mathbf{\Phi}}_\mu(1)\, dv_1, \tag{41}$$

$$e_\mu = \int \bar{\mathbf{\Phi}}^+_\mu(1) \mathfrak{H}'(1) \bar{\mathbf{\Phi}}_\mu(1)\, dv_1 - \int \mathbf{\Phi}^+_\mu(1) \mathfrak{H}'(1) \mathbf{\Phi}_\mu(1)\, dv_1. \tag{42}$$

Here

$$\mathfrak{H}'(1) = F'(1) \cdot \mathbf{1} + \boldsymbol{\sigma} \cdot \boldsymbol{G}'(1), \tag{43}$$

with the form of F' and G' given by (11) but with the density matrix obtained from (30b).

An orbital form of the gap equation is obtained when we make specific choices for the spin orbitals $\bar{\psi}_\mu$. Both the set of reference spin orbitals ψ_μ and the final set of spin orbitals ϕ'_μ should be associated with definite Fukutome classes. Different pairs of such classes will give rise to specific orbital forms of the gap

equation. We derive here some of the cases which are obtained when the set of reference spin orbitals belongs to the TICS class.

This means that

$$\psi_\mu = \begin{cases} (\alpha, \beta)\begin{pmatrix} \chi_k \\ 0 \end{pmatrix}; & \mu = 2k; \\ (\alpha, \beta)\begin{pmatrix} 0 \\ \chi_k \end{pmatrix}; & \mu = 2k+1. \end{cases} \tag{44}$$

We use the convention $N = 2(2n+1)$, so that $-n \leq k \leq n$.

We first consider the case when the determinant D' is of either TICS or CCW type. Then

$$\bar{\psi}_\mu = \begin{cases} (\alpha, \beta)\begin{pmatrix} \bar{u}_k \\ 0 \end{pmatrix}; & \mu = 2k; \\ (\alpha, \beta)\begin{pmatrix} 0 \\ \bar{u}_k \end{pmatrix}; & \mu = 2k+1. \end{cases} \tag{45}$$

In this case

$$\mathfrak{H}'(1) = F'(1) \cdot \mathbf{1}; \tag{46a}$$

$$u_{2k} = u_{2k+1} = \alpha_k; \qquad v_{2k} = v_{2k+1} = \beta_k; \tag{46b}$$

$$\phi'_\mu = \begin{cases} (\chi_k \alpha_k + \bar{u}_k \beta_k)\alpha = a_k \alpha; & \mu = 2k; \\ (\chi_k \alpha_k + \bar{u}_k \beta_k)\beta = a_k \beta; & \mu = 2k+1; \end{cases} \tag{46c}$$

$$\Delta_{2k} = \Delta_{2k+1} = \delta_k = -2 \operatorname{Re} \int \bar{u}_k^*(1) F'(1) \chi_k(1)\, dv_1; \tag{46d}$$

$$e_{2k} = e_{2k+1} = \gamma_k = \int \bar{u}_k^*(1) F'(1) \bar{u}_k(1)\, dv_1 - \int \chi_k(1) F'(1) \chi_k(1)\, dv_1; \tag{46e}$$

and the gap equation reduces to

$$\delta_k = -\frac{1}{2} \sum_l \left\{ \frac{j_{kl}\delta_l}{\sqrt{\gamma_l^2 + \delta_l^2}} + k_{kl}\left[1 - \frac{\gamma_l}{\sqrt{\gamma_l^2 + \delta_l^2}}\right] \right\}, \tag{47}$$

with

$$\begin{aligned} j_{kl} &= J_{2k,2l} + J_{2k,2l+1} \\ &= 2[(\bar{k}k|\bar{l}l) + (\bar{k}k|l\bar{l}) + (k\bar{k}|\bar{l}l) + (k\bar{k}|l\bar{l})] \\ &\quad - (\bar{k}l|\bar{l}k) - (\bar{k}\bar{l}|lk) - (kl|\bar{l}\bar{k}) - (k\bar{l}|l\bar{k}); \end{aligned} \tag{48a}$$

$$\begin{aligned} k_{kl} &= K_{2k,2l} + K_{2k,2l+1} \\ &= 2[(\bar{k}k|\bar{l}\bar{l}) - (\bar{k}l|ll) + (k\bar{k}|\bar{l}\bar{l}) - (k\bar{k}|ll)] \\ &\quad - (\bar{k}\bar{l}|\bar{l}k) + (\bar{k}l|lk) - (k\bar{l}|\bar{l}\bar{k}) + (kl|l\bar{k}). \end{aligned} \tag{48b}$$

Then we consider an ASDW state with ψ_μ given by (44) but with

$$\bar{\psi}_\mu = \begin{cases} (\alpha, \beta)\begin{pmatrix} \bar{u}_k \\ 0 \end{pmatrix}; & \mu = 2k; \\ (\alpha, \beta)\begin{pmatrix} 0 \\ -\bar{u}_k \end{pmatrix}; & \mu = 2k+1. \end{cases} \tag{49}$$

Then

$$\mathfrak{H}'(1) = F'(1) \cdot \mathbf{1} + \sigma_3 G_3'; \tag{50}$$

$$u_{2k} = u_{2k+1} = \alpha_k; \qquad v_{2k} = v_{2k+1} = \beta_k; \tag{51a}$$

$$\phi_\mu' = \begin{cases} (\chi_k \alpha_k + \bar{u}_k \beta_k)\alpha = a_k \alpha; & \mu = 2k; \\ (\chi_k \alpha_k - \bar{u}_k \beta_k)\beta = \bar{a}_k \beta; & \mu = 2k+1. \end{cases} \tag{51b}$$

The extremum conditions (31) imply with (51a)

$$\frac{\Delta_{2k}}{e_{2k}} = \frac{\Delta_{2k+1}}{e_{2k+1}}, \tag{52}$$

but in general there is no other connection between Δ_{2k} and Δ_{2k+1} or e_{2k} and e_{2k+1} separately. As discussed by Berggren and Johansson [15] great care is needed for handling the phase of the gap function.

In many cases the functions $\bar{u}_k$ are however chosen in such a way that further simplifications are possible. The non vanishing component of the spin density is in this case

$$S_3'(1, 1') = \sum_l [\chi_l(1)\bar{u}_l(1') + \bar{u}_l(1)\chi_l(1')]\alpha_l \beta_l. \tag{53}$$

By choosing the $\bar{u}_l$ in a suitable way one can satisfy the conditions

$$\int \chi_k(1) G_3'(1) \chi_k(1)\, dv_1 = \int \bar{u}_k(1) G_3'(1) \bar{u}_k(1)\, dv_1 = 0; \quad \text{all } k, \tag{54}$$

which with (51) and (42) give

$$e_{2k} = e_{2k+1} = \gamma_k. \tag{55}$$

From (52) we then get

$$\Delta_{2k} = \Delta_{2k+1} = \delta_k. \tag{56}$$

If (55) and (56) are satisfied the two spin orbitals $a_k\alpha$ and $\bar{\alpha}_k\beta$ (cf. (51b)) have the same spin orbital energy with respect to the effective Hamiltonian (50).

With the spin orbitals (51b), the integrals $K_{\mu\nu}$ (39), satisfy

$$K_{2k,2l} = -K_{2k+1,2l+1}; \qquad K_{2k,2l+1} = -K_{2k+1,2l}, \tag{57}$$

so that if (54) holds the gap equation reduces to

$$\delta_k = \sum_l \frac{q_{kl}\delta_l}{\sqrt{\gamma_l^2 + \delta_l^2}}, \tag{58}$$

with

$$\begin{aligned} q_{kl} &= -\tfrac{1}{2}(J_{2k,2l} + J_{2k,2l+1}) \\ &= \tfrac{1}{2}[(\bar{k}\bar{l}|\bar{l}k) + (\bar{k}\bar{l}|lk) + (kl|\bar{l}\bar{k}) + (k\bar{l}|l\bar{k})]. \end{aligned} \tag{59}$$

This is the most common form of the gap equation, but we notice that this particular form holds only under certain conditions.

4. Discussion

The general spin orbital forms of the instability conditions and gap equations, that were derived in Refs. 7 and 8, respectively have served as starting points for this paper. Further information about the structure of these expressions require specialization to definite orbital forms, which must be associated with one of the eight classes in Fukutome's classification scheme. These orbital forms constitute the starting points for actual numerical applications.

We have indicated general procedures for going from spin orbital to orbital forms. Some specific examples illustrate simplifications which are possible, but also the delicate connection between the form of the trial functions and the final equations.

Instability studies can be regarded as a preliminary step for obtaining the final solutions. The gap equations are normally solved by iteration and starting values can be obtained from eigenvectors of the "instability matrix" with negative eigenvalues.

Particularly for extended systems it is very desirable to really exploit the gap equation in the search for the best possible solutions of GHF type. We hope that the results presented in this paper will contribute towards that goal.

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Received December 17, 1981