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Commentationes

On Damping in Self-Consistency Cycling Procedures*

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The effects of damping on cycling procedures intended to produce self-consistent results among coupled equations are investigated. Analytic procedures reveal that Hartree damping will effect the rate and mode of convergence without influencing the converged result for general series of polynomials. Other procedures may not meet the latter critical requirement. Choice of damping factor is analyzed and the relevance of geometric series extrapolation techniques to the convergence properties, with and without damping, of coupled polynomial series is examined.

Dämpfungseffekte bei zyklischen Prozeduren, die angewendet werden, um von gekoppelten Gleichungen selbstkonsistente Resultate zu gewinnen, werden untersucht. Analytische Prozeduren offenbaren, daß die Hartree-Dämpfung auf die Schnelligkeit und die Art der Konvergenz wirkt, ohne bei allgemeinen Reihen aus Polynomen das konvergente Resultat dabei zu beeinflussen. Andere Prozeduren brauchen letztere kritische Forderung nicht zu erfüllen. Die Wahl des Dämpfungsfaktors wird analysiert und die Bedeutung der Extrapolationstechniken geometrischer Reihen für die Konvergenzeigenschaften von gekoppelten Reihen von Polynomen, mit und ohne Dämpfung, wird überprüft.

Etude des effets d'amortissement dans les procédés itératifs utilisés pour obtenir des résultats self-consistants pour des équations couplées. Des procédés analytiques montrent que l'amortissement de Hartree effectera la vitesse et le mode de convergence sans pour autant changer le résultat pour des séries générales de polynômes. D'autres procédés peuvent ne pas remplir cette condition critique. Le choix du facteur d'amortissement est analysé et l'on étudie le rôle des techniques d'extrapolation des séries géométriques dans les propriétés de convergence, avec et sans amortissement, pour les séries polynomiales couplées.

Introduction

A widely used computational approach to solve physical system behaviour characterized by non-linear parametric equations involves cycling among these equations until the parameter and the result sets they produce are consistent with each other and with whatever bounds are known for the phenomenon they represent. The SCF procedure as developed for the Hartree-Fock-type matrix eigenvalue problem [1] represents a well-defined and familiar application of this approach in theoretical chemistry. Semi-empirical methods in quantum chemistry have also involved the technique. Self-consistency requirements among diagonal matrix element parameters (α's) and the π-electron charge densities (q's) was introduced as an empiricism some time ago to improve Hückel calculations, especially for ionic species [2]. Subsequent and usually more firmly grounded applications have been made in π-electron theory [3, 4], crystal field theory

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calculations [5], and more recently in the all-electron extended-Hückel [6] and Pople SCF methods [7].

In all of the applications mentioned, and those of a physically unrelated nature as well, there is a possibility and in some cases a likelihood that parameter adjustment between cycles strictly conforming to the determining equations will produce unsatisfactory results. Divergences of an absolute or oscillatory nature may be encountered which lead to no useful result at all. Very slow convergence which yields results only at great computational cost must be judged almost as unsatisfactory. Both may be avoided in some cases by scaling down or damping the cycling corrections with the alternative aims of preventing the overshoot which might lead to an instability (and thence to a divergent condition for the series characterizing a system variable), or hastening an otherwise stable but slowly convergent series. A necessary condition which of course must be satisfied by the damping method is that it does not substantially alter the position while improving the mode of convergence. This is not a matter of such serious concern in "exact calculations" where bounds such as are provided by the variational principle may be recognized. It is with this question of forms of damping and their effects on mode and position of convergence for some typical cases of self-consistency cycling in semi-empirical MO calculations where no such external bounds exist that the present work deals. How geometric series extrapolation techniques simulate the behaviour of converging series and how they may resolve the problems encountered in series which diverge upon cycling are also examined.

Coupled Equation Systems

The set of input parameters, or variables explicitly dependent upon such parameters (designated as α's), determine in the cases of present interest a set of dependent variables (q's) through matrix (secular) equations

$$q_\mu^{(1)} = f_\mu(\alpha_1^{(0)}, \alpha_2^{(0)}, \ldots, \alpha_n^{(0)}) . \tag{1}$$

In turn, relations are derived in a manner consistent with the empiricism employed for the secular equation variables as functions of the output q-values

$$\alpha_i^{(1)} = F_i(q_1^{(1)}, q_2^{(1)}, \ldots, q_m^{(1)}) . \tag{2}$$

Superscripts in Eqs. (1) and (2) denote cycle numbers. Repetition of the process is continued until the values of q obtained in a given cycle are consistent with the values of α they determine and are determined by, or, in practice by testing values of q which do not change by more than a prespecified amount from the q-results obtained in the previous cycle.

With the understanding that, in the absence of cross-terms in the independent variables, Eqs. (1) and (2) may be recast, viz.,

$$q_\mu^{(t)} = f_{1\mu}(\alpha_1^{(t-1)}) + f_{2\mu}(\alpha_2^{(t-1)}) + \cdots + f_{n\mu}(\alpha_n^{(t-1)}) \tag{3}$$

$$\alpha_i^{(t)} = F_{1i}(q_1^{(t)}) + F_{2i}(q_2^{(t)}) + \cdots + F_{mi}(q_m^{(t)}) , \tag{4}$$

and that the sums of terms over the functions f and F introduce no additional complications over those encountered where dependence on the single variables,

$\alpha_1 = \alpha$ and $q_1 = q$, is assumed, the following analysis may be made. Cross-terms in the independent variables, normally present in physical systems of more than the simplest or most highly symmetrical nature [8] may in approximation be replaced when cycling changes are small by first-order derivative expansions.

1. Linear Parametric Equations

In the simplest cases where both dependent cycling variables are linear functions of the independent variables, i.e., $\alpha = \omega q + a$, $q = S\alpha + b$, it is apparent that

$$\begin{aligned} \Delta\alpha_t &\equiv \alpha_t - \alpha_{t-1} = \omega \Delta q_t \,, \\ \Delta q_{t+1} &\equiv q_{t+1} - q_t = S\omega \Delta q_t \,, \end{aligned} \tag{5}$$

and, therefore,

$$\Delta q_{t+1} = (S\omega)^t \Delta q_1 \,. \tag{6}$$

Note, cycle number is now represented by subscript to simplify notation. Since,

$$\begin{aligned} q_t &= \sum_{j=1}^{t} \Delta q_j + q_0 \,, \\ q_{t+1} &= \Delta q_1 \sum_{j=0}^{t} (S\omega)^j + q_0 \\ &= \Delta q_1 \left\{ \frac{(S\omega)^{t+1} - 1}{(S\omega) - 1} \right\} + q_0 \,. \end{aligned} \tag{7}$$

In the limit where $t \to \infty$ and $|S\omega| < 1$,

$$\begin{aligned} q_\infty - q_0 &= \Delta q_1 / (1 - S\omega) = \frac{b + Sa}{1 - S\omega} - q_0 \,, \\ \alpha_\infty - \alpha_0 &= \omega \Delta q_1 / (1 - S\omega) \,. \end{aligned} \tag{8}$$

The cycling scheme here generates a geometric series; in the event the absolute value of $S\omega$ is equal to unity oscillatory behaviour is noted, and if greater than unity the series diverges. Assumption of convergent geometric series behaviour, it is useful to note, is often made for complex cycling relations as an extrapolation technique to hasten slow convergence. The results of three cycles are employed to generate "extrapolated" values for the variables of interest, which are then themselves resubmitted to the cycling procedure for further efforts toward reaching convergence. If necessary, the extrapolation procedure is reemployed after the results of several conventional cycles are obtained, constituting a second, approximate cycling – within – a cycling procedure [9]. See further discussions below on correspondence to extrapolation procedures.

To return to the cases of immediate interest, for $|S\omega| \lesssim 1$, damping procedures which retard divergence or hasten convergence are desirable. A method suggested by Hartree [10] where input for cycle $t+1$ (the α value as usually construed) is constructed as,

$$(\text{Input})_t + D[(\text{Output})_{t+1} - (\text{Input})_t]$$

is relevant and may be shown to have the following interesting properties. In the present notation, the equation sequence which pertains is,

$$\Delta q_{t+1} = S \Delta \alpha_t \,,$$

as before, and,

$$\begin{aligned}
\alpha_1 &= \alpha_0 + D(a + \omega q_1 - (a + \omega q_0)) = \alpha_0 + D\omega\, \Delta q_1\,, \\
\alpha_2 &= \alpha_1 + D(a + \omega q_2 - (a + \omega q_0 + D\omega\, \Delta q_1)) \\
&= \alpha_1 + D(\omega(q_2 - q_0) - D\omega\, \Delta q_1) \\
&= \alpha_1 + D\omega(\Delta q_2 + (1 - D)\, \Delta q_1)\,, \\
\alpha_3 &= \alpha_2 + D\omega(\Delta q_3 + (1 - D)\, \Delta q_2 + (1 - D(2 - D))\, \Delta q_1) \\
&\;\;\vdots \qquad\qquad\qquad\qquad \vdots
\end{aligned} \tag{9}$$

$$\alpha_t = \alpha_{t-1} + D\omega \sum_{j=0}^{t-1} (1 - D)^j\, \Delta q_{t-j}\,, \tag{10}$$

$$\Delta q_{t+1} = DS\omega \sum_{j=0}^{t-1} (1 - D)^j\, \Delta q_{t-j}\,.$$

Since the recurrence relation,

$$\begin{aligned}
\Delta q_{t+1} &= (1 - D + SD\omega)\, \Delta q_t\,, \qquad t > 1\,, \\
\Delta q_2 &= SD\omega\, \Delta q_1
\end{aligned} \tag{11}$$

may be shown to hold, reduction to the first cycle difference and expansion of Δq_t as in Eq. (7) results in,

$$\Delta q_{t+1} = SD\omega(1 - D + SD\omega)^{t-1}\, \Delta q_1\,, \tag{12}$$

$$q_t - q_0 = \Delta q_1 + SD\omega\, \Delta q_1 \sum_{j=0}^{t-2} (1 - D + SD\omega)^j\,. \tag{13}$$

Geometric series summation leads to,

$$q_t - q_0 = \Delta q_1 \left\{ 1 + \frac{SD\omega[(1 - D + SD\omega)^{t-1} - 1]}{(1 - D + SD\omega) - 1} \right\}. \tag{14}$$

In the limit $t \to \infty$, for $|1 - D + SD\omega| < 1$,

$$q_\infty - q_0 = \Delta q_1 \left\{ \frac{D}{D - SD\omega} \right\} = \frac{\Delta q_1}{1 - S\omega} = \frac{Sa + b}{1 - S\omega} - q_0 \tag{15}$$

which is identical to the result which would have been obtained without damping. This is a necessary outcome if the results obtained with damping are to be considered trustworthy. The parameter limits within which cycling convergence is guaranteed are now extended. For $S\omega$ negative, as it usually would be in semi-empirical quantum chemical applications, $0 < D < 2/(1 - S\omega)$ will guarantee convergence in the cycling procedure. Interestingly, if D is greater than $(1 - S\omega)^{-1}$, oscillatory progress toward convergence would be observed, if less than this quantity, monotonic asymptotic behaviour would be noted. The maximum rate of convergence is obtained when D is equal to this fraction as combination of Eqs. (14) and (15) to obtain $(q_\infty - q_t)$ reveals. The cycle 2 results yields q_2 equal to q_∞. This agrees

with intuition as regards to the behaviour expected on cross-over between oscillatory and monotonic progressions.

For $S\omega$ between zero and -1, damping is of course not necessary but could aid in the rate of convergence. For $S\omega$ positive but less than unity, damping is not required and as a matter of fact could only be helpful by being an amplification factor ($D > 1$). For $S\omega$-values greater than unity, only a negative and thereby physically unrealistic value of D could prevent divergence upon cycling.

Other damping procedures may be devised. One which appears superficially attractive recognizes the change (per cycle) in the variable q and scales down the change in α in the following simple proportional fashion to Δq,

$$\begin{aligned} \Delta q_{t+1} &= S\,\Delta\alpha_t \\ \alpha_{t+1} &= \alpha_t + D\omega\,\Delta q_{t+1} \end{aligned} \tag{16}$$

This procedure may quickly be shown capable of producing a convergent result which however is dependent upon D. In fact, transforming $D\omega$ of Eq. (16) to ω of Eqs. (5) and following the development through Eq. (8) results in,

$$q_\infty - q_0 = \Delta q_1/(1 - DS\omega) \tag{17}$$

convergent for $|DS\omega| < 1$. Therefore while the convergence properties may be improved by damping, the converged and as well as all intermediate results are unreliable because of their D-dependence. Damping, it should be recognized, will always affect intermediate cycle results, even when disappearing in the convergent results (cf., Eqs. (9–15)). Attempting to attach any physical reality to intermediate results forthcoming from a cycling procedure would as a result seem futile.

It is pertinent at this point to recognize the self-consistency procedures which make use of paths of descent (e.g., path of steepest descent) are also damping procedures, although not as obvious in application. As often employed [11], the initial estimate of the eigenvectors obtained from the descent method is used to adjust the Hamiltonian matrix, thereby condensing the cycling to a single from a two stage operation. This method falls beyond the scope of the present analysis; we are here concerned with the stage of Hamiltonian adjustment under the assumption that the eigenvectors are immediately available, either from an analytic polynomial in the model calculations, or otherwise from conventional diagonalization techniques.

2. Coupling in a Quadratic Equation System

Recently adopted variations of extended Hückel theory invoking diagonal matrix element adjustment and self-consistency cycling have assumed quadratic parametric dependences (on q, for the valence state ionization potentials which are equated to the α-values [6, 12]). If linear dependence of q upon α in the single variable approximation is again employed as the convenient, potentially analyzable system for examination, and the Hartree damping procedure adopted, the following analysis may be made.

$$
\begin{aligned}
\Delta q_{t+1} &= S\,\Delta\alpha_t\,,\\
\alpha_1 &= \alpha_0 + D\,[a+\omega q_1+\omega' q_1^2-(a+\omega q_0+\omega' q_0^2)]\\
&= \alpha_0 + D(\omega\,\Delta q_1+\omega' Q_1\,\Delta q_1)\,,\\
\alpha_2 &= \alpha_1 + D\{\omega[(1-D)\,\Delta q_1+\Delta q_2]+\omega'[(Q_2-DQ_1)\,\Delta q_1+Q_2\,\Delta q_2]\}\\
&\;\;\vdots \qquad\qquad\qquad\qquad \vdots\\
\alpha_t &= \alpha_{t-1} + D\left\{\omega\sum_{j=0}^{t-1}(\hat{1}-D)^j\,\Delta q_{t-j}\right.\\
&\qquad \left.+\omega'\left[\sum_{j=0}^{t-1}\left(Q_t+\sum_{l=1}^{j}(-D)^l\sum_{k=0}^{j-l}\binom{j-k-1}{j-k-l}Q_{k+t-j}\right)\Delta q_{t-j}\right]\right\}.
\end{aligned}
\tag{18}
$$

Here $Q_t = q_t + q_0$ and the coefficient of Q inside the k-sum is the binomial coefficient. Exchange of the order of summation (k and l indices) and recognition of known sums over binomial series [13] yields for the general case,

$$
\alpha_t = \alpha_{t-1} + D\left\{\omega\sum_{j=0}^{t-1}(1-D)^j\Delta q_{t-j}+\omega'\sum_{j=0}^{t-1}\left(Q_t-D\sum_{k=0}^{j-1}Q_{k+t-j}(1-D)^{j-k-1}\right)\Delta q_{t-j}\right\}.
\tag{19}
$$

The recurrence relationship between the successive cycle results for Δq which may be obtained from the first and last of Eqs. (18) similar to Eq. (11), is,

$$
\begin{aligned}
\Delta q_{t+1} &= (1-D+SD[\omega+\omega' Q_t])\,\Delta q_t\\
&= \left(1-D+SD\left[\omega+2\omega' q_0+\omega'\sum_{j=1}^{t}\Delta q_j\right]\right)\Delta q_t\,, \qquad t>1\,,\\
\Delta q_2 &= SD(\omega+\omega' Q_1)\,\Delta q_1\,.
\end{aligned}
\tag{20}
$$

Despite what appears to be a much more complicated dependence for the intermediate and converged values of q_t, it may be shown most conveniently by summation over the first of Eq. (20) that in the limit,

$$
q_\infty - q_0 = \frac{\Delta q_1}{1-S[\omega+\omega'(q_\infty+q_0)]} = \frac{Sa+b}{1-S[\omega+\omega' q_\infty]} - q_0\,,
\tag{21}
$$

which are analogous equations in form, at least as far as the lack of D dependence goes, to those obtained in the previous case. Solution to obtain the converged value of q is of course most expeditiously accomplished through the quadratic which may be generated from Eq. (21). For small ω' $\left(\text{i.e., } |\omega'| \ll \left|\frac{(1-S\omega)^2}{4S(Sa+b)}\right|\right)$,

$$
q_\infty \cong \frac{(Sa+b)}{1-S\omega}\left(1+\frac{S\omega'(Sa+b)}{(1-S\omega)^2}\right).
\tag{22}
$$

This expansion reveals ω' will cause an essentially linear perturbation on the converged value of q under the particular circumstances that $S\omega$ is positive and small (smaller than 2) and $S(Sa+b)$ is not appreciably smaller in magnitude than unity. Semi-empirical quantum chemical applications should however usually require the original unexpanded quadratic form arising from Eq. (21).

The convergence properties of the cycling system are usefully examined at this point and compared to those obtained for the linear system. Eq. (20) reveals that for absolute convergence of the series in q, after the first term,

$$|1 - D + SD[\omega + \omega' Q_t]| < 1 \tag{23}$$

and hence that for D positive, for convergence,

$$D < \frac{2}{1 - S[\omega + \omega' Q_t]}, \tag{24}$$

The ω' term will then be the cause of whatever convergence property differences may exist from those outlined in detail above for the linear systems. For the systems which will require damping, i.e., where $(S\omega + S\omega' Q_t)$ less than -1, convergence can only be guaranteed if the appropriate extremum value of Q_t which would be encountered in the cycling process is employed in Eq. (24). That is, the maximum absolute value of Q_t where $S\omega' Q_t$ is positive, or the minimum absolute Q_t if $S\omega' Q_t$ is negative will be required. If D is constrained to be smaller than $(1 - S[\omega + \omega' Q_t])^{-1}$, monotonic convergence is guaranteed and the choice of the extremum Q_t value is thereby restricted to those generated from the second cycle (q_2) or the converged value (q_∞).

In practice, the latter is of course not available; q_2 or a value larger or smaller by a small increment than q_3, depending upon the direction dictated by the first three damped cycles, could be used as a first estimate for determining D in a process of trial and error. The trial and error process for this estimation resembles that which would be required for obtaining q_∞ from Eq. (21). The rate at which the cycling procedure could produce a converged value makes the choice of D in systems which approximate those chosen here for closed form analysis a matter of practical as well as pedagogic concern.

In a manner similar to the analysis of the dependence of rate of convergence on D in the linear cases considered, it may be concluded that maximum convergence will occur for D equal to $(1 - S[\omega + \omega' Q_\infty])$. At this value there will be crossover in mode of progression (between oscillatory and monotonic), and, again, q_2 will be equal to q_∞, with all Δq_t, for $t > 2$, equal to zero.

3. Higher Order Equation Systems

The analytic procedure followed in the preceding coupled equation systems apparently is capable of extension to higher order sets, however, not without considerable and algebraically involved efforts. Rather than attempting to obtain generalized solutions in this manner, a digital computer program was constructed to test polynomials up to order 6 for both equations. A variety of polynomial coefficient combinations were tested. From the results obtained it was ascertained that the Hartree damping procedure generally has no effect on the converged results, independent of the orders of the polynomials, while influencing the rate of convergence and the ability to converge upon cycling. Table 1 records a typical set of results for linear, quadratic and cubic equation combinations as obtained directly from the computer.

These results tend to bear out the earlier conclusions concerning the effect of D on the rate of convergence. Cases which are divergent upon cycling without damping ($D = 1.0$) are often made to converge with D not very different from unity and, in the cited polynomials at least, can always be made to converge with somewhat stronger damping. Further, convergence is always found to be hastened

Table 1. *Convergence properties for coupled polynomial equations*[a]

α[c]	q[b,d] $S = -0.2$	$S' = 0.005$	$S'' = -0.0002$
$\omega = 5.0$	0.1500000	0.3252907	0.3701462
	$d, 35, 13, \overline{12}$	$d, 257, 24, \overline{7}$	$d, d, 32, 8$
$\omega' = -3.0$	0.1574358	0.3747873	0.4428755
	$81, 23, 9, \overline{15}$	$70, 21, \overline{9}, \overline{16}$	$61, 18, \overline{8}, \overline{16}$
$\omega'' = 2.0$	0.1565880	0.3599824	0.416580
	$99, 24, 10, \overline{14}$	$d, 39, 13, \overline{12}$	$d, 56, 16, \overline{10}$

[a] Entries are within each block the converged value of q, verified to be independent of D, and the number of iterations required for convergence to $|q_t - q_{t-1}| < 10^{-7} q_t$ with D values of 1.0, 0.8, 0.6 and 0.4. The polynomials of higher order contain the lower order terms which precede them in the particular column and row. Note, a bar over the iteration number indicates monotonic progress toward convergence, over the early part of the series at least , and d indicates divergence.

[b] The constant coefficient b is -1.7.

[c] The constant coefficient a is -10.0.

[d] The S-primed values are the coefficients for the higher order (than linear) terms in the dependence of q upon α.

by damping, suggesting all the polynomial combinations examined behave in a similar manner to the linear- and quadratic-α polynomials with linear-q cases discussed in detail previously.

In fact, from examination of these and similar results in combination with the analytic details obtained above, it appeared that the general expression for converged q for polynomials of any order in q and α should be,

$$q_\infty = \frac{b + a\left(\dfrac{q_\infty - b}{\alpha_\infty}\right)}{1 - \left(\dfrac{q_\infty - b}{\alpha_\infty}\right)\left(\dfrac{\alpha_\infty - a}{q_\infty}\right)}. \tag{25}$$

This equality, which may be easily verified by multiplying the quotient out and expanding the product terms, quickly yields the polynomial in q_∞ when substitution for α_∞ in terms of q_∞ is made, and hence, upon solution of the resultant polynomial equation, yields the desired value of q_∞. By analogous reasoning to that employed above, it is easily ascertained that for the cases examined in Table 1 the improvement in the rate of convergence with D values somewhat less than unity occurs because

$$\left(1 - \left(\frac{q_\infty - b}{\alpha_\infty}\right)\left(\frac{\alpha_\infty - a}{q_\infty}\right)\right)^{-1}$$

will always be roughly around 1/2. The leading and most important terms $(1-S\omega)^{-1}$ yield a crossover point for mode of progression and consequently the most potent choice of D, as regards convergence rate, at precisely 1/2.

Other interesting analysis is possible; e.g., on how a series which begins to converge monotonically can change its mode to oscillatory as cycling continues (see the effects of Q_t, for example in the quadratic case discussed in detail above). The most important implication of the general results appears however to concern the general efficacy of the Hartree procedure. It would appear from the results obtained that Hartree damping will always produce cycling results if convergent which are independent of the damping factor employed, at least in cases of pairs of single variables (one α dependent on one q and *vice versa*). The functional dependence will not matter since most functions of general interest may be expanded in terms of an appropriate convergent polynomial series for which the present analysis pertains.

Relevance to Extrapolation Procedures

As implied above, an extrapolation procedure which employs the results of three successive cycles and assumes a geometric series relationship among them [14] will approximate the remainder of the progression to which it is applied exactly as that of a coupled bilinear system. Since geometric series extrapolation procedures are often used, the implications of this fact are usefully pursued. To the extent which coupled higher order polynomials resemble the bilinear system in mode of convergence, extrapolation may be expected to hasten convergence rate. Moreover, even in apparently divergent cases, reverse or back-extrapolation, similar in form to the normal procedure and entirely justifiable within the geometric series approximation, can often provide a new and effective base point from whence continued iteration can lead to a convergent self-consistent set of results.

From Eq. (20) for the quadratic (α equation) case, it is apparent that the error accompanying extrapolation will depend directly upon the $SD\omega' Q_t$ term: if Q_t is relatively constant, or the entire term is relatively small, geometric series extrapolation can be expected to yield a satisfactory estimate of the converged value of q. For the cycled system which converges, the further along the extrapolation procedure is applied, the closer the extrapolated value should be to the converged value. Of course, on the other hand, the earlier the extrapolation is used, the greater the potential saving in computational effort. Such conclusions are general; how they apply in detail in the cases of the higher polynomials and hence how they may be expected to apply to functions of general interest may be better understood from the results contained in Table 2. The polynomials are just those which were chosen for detailed examination in Table 1.

It is clear from an examination of Table 2 that geometric series extrapolation is effective in hastening convergence, even for coupled series which exhibit appreciable deviation from the bilinear form. Further, when compared with Table 1, it is not surprising to find that damping which speeds the rate of convergence upon cycling likewise improves the precision with which the extrapolated values from the first three iterations approximate the conventionally obtained convergent results. This is also reflected in the other Table 2 entries, i.e., the earliest cycle from which extrapolation yields the converged value within 10^{-6}.

Table 2. *Geometric extrapolation effects on coupled polynomial equations*[a,b]

α	q $S=-0.2$	$S'=0.005$	$S''=-0.0002$
$\omega = 5.0$	0.150000	0.325291	0.370146
	0.150000,1	*0.358103*,1	*0.515056*,1
	0.150000,1	0.329161,54	*0.391618*,1
	0.150000,1	0.325106,4	0.369726,5
	0.150000,1	0.325291,1	0.370141,2
$\omega' = -3.0$	0.157436	0.374787	0.442876
	0.160517,20	0.389613,18	0.450396,15
	0.157894,5	0.375590,5	0.442892,2
	0.157437,1	0.374856,2	0.442662,2
	0.157247,3	0.369384,4	0.424370,5
$\omega'' = 2.0$	0.156588	0.359982	0.416580
	0.159175,23	*0.389256*,1	*0.450380*,1
	0.157024,5	0.367787,10	0.437561,15
	0.156591,2	0.360273,3	0.418077,4
	0.156492,3	0.359928,2	0.416580,1

[a] Entries are within each column block, the converged value of q, and, for the series damped with D values 1.0, 0.8, 0.6 and 0.4 respectively, the q-value obtained by extrapolation with q_1, q_2 and q_3, followed by the smallest value of t from which extrapolation employing q_t, q_{t+1} and q_{t+2} approximates q_∞ to the 6 place accuracy shown. For divergent progressions, the back-extrapolated value, using q_1, q_2 and q_3 which is generally the best possible combination, is indicated by italics.

[b] Footnotes b, c, and d of Table 1 pertain.

Interestingly, extrapolation in the damped series which are monotonically convergent is not generally more precise than in the differently damped series (with the same polynomials) which oscillate in progress to convergence. In Table 1, the monotonic series generally converged more rapidly.

Back extrapolation, most effective when applied to the earlier cycle results, before very wide swings are encountered, is generally able to approximate the self-consistent value of a series as well as conventional cycling in convergent series can within the first 20% of the total cycles required. Recycling from these back-extrapolated points often results in convergent series. Occasionally, however, more than one back extrapolation may be required before this outcome is achieved.

Conclusions

It is apparent from the foregoing analysis that damping procedures may be extremely useful in hastening the rate of convergence or preventing divergence in self-consistency cycling procedures, but care must be exercised to avoid having the damping affect the final or convergent result. The procedure suggested by Hartree is apparently sound in both these regards. Coupled polynomial equations of any order are shown analytically not to exhibit functional dependence of their convergent results upon damping in this procedure. In fact, if damping effects are ever to be noted with this method, these could only arise in the multi-variable cases because of cross-terms between or among these variables. Extension of the

analysis reveals that geometric series extrapolation methods simulate the behaviour of coupled equations in terms of the behaviour of the simplest coupled system, the bilinear equation system. How well the approximation does is of course dependent on the polynomial system; tests reveal its general utility in speeding convergence and for that matter in reversing trends toward divergence. Damping procedures when coupled with extrapolation techniques are shown to be especially effective in decreasing the computational efforts required in self-consistency calculations, more effective than either may be alone.

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