Simultaneous multigrid techniques for nonlinear eigenvalue problems: Solutions of the nonlinear Schrödinger-Poisson eigenvalue problem in two and three dimensions

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Algorithms for nonlinear eigenvalue problems (EP's) often require solving self-consistently a large number of EP's. Convergence difficulties may occur if the solution is not sought in an appropriate region, if global constraints have to be satisfied, or if close or equal eigenvalues are present. Multigrid (MG) algorithms for nonlinear problems and for EP's obtained from discretizations of partial differential EP have often been shown to be more efficient than single level algorithms. This paper presents MG techniques and a MG algorithm for nonlinear Schrödinger-Poisson EP's. The algorithm overcomes the above mentioned difficulties combining the following techniques: a MG simultaneous treatment of the eigenvectors and nonlinearity, and with the global constraints; MG stable subspace continuation techniques for the treatment of nonlinearity; and a MG projection coupled with backrotations for separation of solutions. These techniques keep the solutions in an appropriate region, where the algorithm converges fast, and reduce the large number of self-consistent iterations to only a few or one MG simultaneous iteration. The MG projection makes it possible to efficiently overcome difficulties related to clusters of close and equal eigenvalues. Computational examples for the nonlinear Schrödinger-Poisson EP in two and three dimensions, presenting special computational difficulties, that are due to the nonlinearity and to the equal and closely clustered eigenvalues are demonstrated. For these cases, the algorithm requires $O(qN)$ operations for the calculation of q eigenvectors of size N and for the corresponding eigenvalues. One MG simultaneous cycle per fine level was performed. The total computational cost is equivalent to only a few Gauss-Seidel relaxations per eigenvector. An asymptotic convergence rate of 0.15 per MG cycle is attained.

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I. INTRODUCTION

Multigrid (MG) techniques for nonlinear problems and for eigenvalue problems (EP's) such as many large scale problems from physics, chemistry, and engineering have often been shown to be more efficient than single level techniques [1–4]. MG techniques can use efficiently features which are generally not used by single level techniques; for example, the problems can be approximated on several discretization levels, the solutions can be well approximated by solutions of coarse level problems, only a few eigenvalues and eigenvectors are sought, and the solutions are dominated by smooth components [2]. Moreover, MG eigenvalue techniques have powerful solving capabilities, for example, they can approximate well the efficient inverse power iteration for eigenvalue problems [5].

MG techniques involve, in general, the processing of the problem on a sequence of discretization levels. Usually, these levels are finite dimensional function spaces defined on increasingly finer grids [3,4].

To treat nonlinear problems or systems of coupled problems, as in our case, algorithms often involve a large number of self-consistent iterations. The iterations may be inefficient or may not converge if the approximated solution is not in an appropriate region. The treatment of these difficulties becomes harder when combined with eigenvalue difficulties. Large computational difficulties are faced by eigenvalue solvers especially when close or equal eigenvalues are present, common difficulties for Schrödinger and electromagnetism EP's. In such cases, instead of approximating an eigenvector, procedures usually approximate a linear combination of eigenvectors with close or equal eigenvalues. This is referred to as eigenvector mixing. See [6] for more discussions on difficulties related to MG eigenvalue solvers for linear EP's. The nonlinear Schrödinger EP treated in the computational examples is ill posed when defined on incomplete clusters of eigenvectors. Global constraints imposed on the solutions, such as norms, orthogonality, and given average, introduce additional difficulties in MG algorithms since these constraints are not conserved by interlevel transfers of solutions, e.g., the transfers alter the norms and orthogonality of solutions.

The above mentioned difficulties are closely coupled. The treatment of the nonlinearity and of the constraints should be done simultaneously with the update of eigenvectors, to keep the approximate solution in the appropriate region of the exact solution where the algorithm is efficient. These motivate a further simultaneous MG approach.

This paper focuses on MG techniques for overcoming the above mentioned difficulties, and presents a MG robust and efficient algorithm for the calculation of a few eigenvalues and their corresponding eigenvectors for the nonlinear Schrödinger-Poisson EP. This problem is important for semiconductor technology. For a theoretical analysis see, for example, [7].

The problem used for illustration is the computation of the first q eigenvectors $u^1, ..., u^q$ and the corresponding smallest eigenvalues (in modulus) $\lambda_1, ..., \lambda_q$ of the discretized Schrödinger-Poisson nonlinear EP (or of Hartree-Fock type)

$$\begin{aligned} \Delta u^i - (V + \epsilon W)u^i &= \lambda_i u^i, \quad i = 1, \ldots, q, \\ \Delta W &= -c_1 \sum_{i=1}^{q} (u^i)^2 + c_2, \\ \|u^i\| &= 1, \\ \int W &= 0. \end{aligned} \tag{1}$$

Periodic boundary conditions are assumed. Eigenvectors in degenerate eigenspaces are required to be orthogonal. The problem has to be solved in two and three dimensions (2D and 3D). V is a given linear potential operator, W is a nonlinear potential, also to be calculated, and c_1, c_2, and ϵ are constants. If ϵ is zero the problem is linear, otherwise it is nonlinear since the potential W depends on the solutions. It is assumed that the clusters containing the desired q eigenvectors are complete.

The problem is represented and solved on a sequence of coarse to fine levels. The algorithm is based on separation of eigenspaces and of eigenvectors in eigenspaces, simultaneously treated with the nonlinearity and the constraints on all levels. Transfers between levels are used to reduce as much as possible the heavy computational tasks from fine levels to inexpensive tasks on coarse levels. The algorithm may be outlined by three steps: (1) get an approximation of the solution on a coarse level; (2) interpolate the solution to a finer level; (3) improve the fine solution by a few MG cycles. Repeat steps 2 and 3 until the finest level is reached. The approximation on the coarse level at step 1 solves first the linear problem ($\epsilon = 0$), then the nonlinear one by a continuation procedure. A MG cycle at step 3 starts on the fine level, transfers the problem successively down to coarser levels and then up, returning to the fine level. On each level, the eigenvectors and the nonlinear potential are updated, and on a coarse level the eigenvectors are separated by projections and backrotations. The separation of fine level eigenvectors by transfers coupled with coarse level projections is called *multigrid projection* (MGP) [8,6].

Simultaneous MG schemes reduce the many self-consistent iterations to solve the nonlinearity to a single simultaneous iteration. Due to the MGP, the algorithm achieves a better computational complexity and a better convergence rate than previous MG eigenvalue algorithms which use only fine level projections. Increased robustness is obtained due to the MGP coupled with backrotations, and due to the simultaneous treatment of eigenvectors with the nonlinearity and with the global constraints.

The presented techniques are applicable to a much larger class of problems, as can easily be observed. In particular, the algorithms without the treatment of nonlinearity were used for linear eigenvalue problems too; see [9,6].

The computational examples were chosen to include special difficulties such as very close and equal eigenvalues. The algorithm uses a few (1–4) fine level cycles, and in each cycle two fine level Gauss-Seidel relaxations per eigenvector are performed. The algorithm yields accurate results for very close eigenvalues, and accuracy of more than ten decimal places for equal eigenvalues. Exact orthogonality of fine level eigenvectors is obtained by the coarse level MGP. A second order approximation is obtained in $O(qN)$ work, for q eigenvectors of size N on the finest level. An asymptotic convergence rate of 0.15 per MG cycle is obtained.

For early works, theory, and more references on MG eigenvalue algorithms, we refer to [10,11,5,2,3,12,4,13]. The sequential MG algorithm for linear EP's, which performs the separation of eigenvectors on the finest level [2], is combined with a conjugate residual method, and applied to a Hartree-Fock nonlinear eigenvalue problem in [14]. In [14] real problems are solved. Our numerical approach differs from the approach in [14] by the MG simultaneous treatment of the nonlinear problem, by the MGP, and by the MG stable subspace continuation techniques.

Previous versions of the results presented here and additional technical discussions are given in the reports [8] and [15]. The linear adaptive techniques presented in [16,6], can be directly combined with the presented techniques. Algorithms and more references for single level large scale complex eigenvalue problems can be found in [17]. We refer to [18–20], for theory on algebraic eigenvalue problems; and to [21–23], for aspects of the single level technique used here, of obtaining a few eigenvectors and their eigenvalues for linear EP's.

The MG projection and backrotations were first introduced in [24], and in the reports [8] and [16], and analyzed in [25]. A related computational approach is outlined in [26].

The paper is organized as follows. The next two subsections I A and I B describe the MG discretization of the nonlinear Schrödinger-Poisson EP and the general full approximation scheme (FAS) interlevel transfers. Section II outlines the MG eigenvector separation techniques presented in more detail in [16,6]. Section III presents the MG nonlinear techniques, i.e., the MG cycle for the nonlinear potential W, the simultaneous updating of eigenvectors and potential, the treatment of global constraints, the subspace continuation procedures, and the full multigrid (FMG) nonlinear eigenvalue algorithm. Sec. IV presents computational examples. Conclusions are presented in Sec. V.

A. The discretization of the nonlinear Schrödinger-Poisson eigenvalue problem

Assume that Ω is a domain in R^d, and let $G_1, G_2, ..., G_m$ be a sequence of increasingly finer grids

that extend over Ω. The space of functions defined on grid G_k is called level k. I_k^l denote transfer operators from level k to level l, e.g., I_k^l can be interpolation operators. The discretization of problem (1), on finest grid G_k, has the following form:

$$\begin{aligned} &\Delta_k u_k^i - (V_k + \epsilon W_k) u_k^i = \lambda_i u_k^i, \\ &\Delta_k W_k = -c_1 \sum_{i=1}^{q} (u_k^i)^2 + c_2, \\ &\|u_k^i\|_k = 1, \\ &\sum W_k^j = 0. \end{aligned} \tag{2}$$

If G_k is not the finest grid then relations (2) include FAS right hand sides as shown in the next sections. Here Δ_k is a discrete approximation to the Laplacian. On the finest level, the eigenvectors in degenerate eigenspaces should be orthogonal. Periodic boundary conditions are assumed for Ω—a box in R^d. The W_k^j denotes the jth component of W_k on level k and V_k is a representation of the potential V on level k, e.g., is a transfer of the finest level V_m to coarser level k, i.e., $V_k = I_m^k V_m$.

B. FAS transfers

The following is a general formulation of the FAS [1], which is applied to the eigenvalue equations, to the separation of eigenvectors, to the nonlinear equation, and to the global constraints. We use the notations from [6]. Assume that

$$F_i U_i = T_i \tag{3}$$

is a level i problem, where F_i is a general operator and T_i is a right hand side. A level j problem

$$F_j U_j = T_j \tag{4}$$

is called a FAS transfer of the level i problem (3) if

$$T_j = I_i^j (T_i - F_i U_i) + F_j I_i^j U_i \ . \tag{5}$$

The level j problem (4) is used in solving the level i problem (3), i.e., in correcting the level i solution U_i^{old} with the level j solution U_j by the FAS correction

$$U_i^{new} = U_i^{old} + I_j^i (U_j - I_i^j U_i^{old}) \ . \tag{6}$$

Assume that U_i is the exact solution of (3). Then the transfer of U_i to level j, $I_i^j U_i$, is the exact solution of (4), and the correction (6) does not change the exact solution U_i.

II. MULTIGRID SEPARATION TECHNIQUES

The introduced algorithm combines MG linear eigenvalue techniques with techniques for nonlinear problems. The linear eigenvalue techniques consist in approximating and separating the desired clusters by relaxations and by MG cycles; and in separating the eigenvectors inside the clusters by MG projections (MGP's). If the eigenvalues are well enough approximated then relaxations and MG cycles also efficiently separately eigenvectors even for clusters of close but not equal eigenvalues. The MGP, the central eigenvector separation tool, introduced and applied in [8,6], is presented briefly next to make the further presentation more clear and self-contained.

Consider the level i eigenvalue relation

$$A_i V_i = V_i \Lambda \ , \tag{7}$$

where $\Lambda = \mathrm{diag}(\lambda_1, \ldots, \lambda_q)$ contains on the diagonal the q sought eigenvalues corresponding to the sought eigenvectors of the matrix A_i, which are the columns of V_i. Assume that U_i which satisfies

$$V_i = U_i E \tag{8}$$

is given instead of V_i, where E is a $q \times q$ invertible matrix to be found. Substituting (8) into (7) gives

$$A_i U_i E = U_i E \Lambda \ . \tag{9}$$

Consider (9) written as a level i problem in FAS form, where $T_i = 0$:

$$A_i U_i E - U_i E \Lambda = T_i E \ . \tag{10}$$

Then the FAS transfer of (10) to level j is

$$A_j U_j E - U_j E \Lambda = T_j E \ , \tag{11}$$

where $U_j = I_i^j U_i$. $T_j E$ is computed by (5), and results in

$$T_j = I_i^j (T_i - A_i U_i) + A_j I_i^j U_i \ . \tag{12}$$

Solutions E and Λ for (11) can be computed by a Rayleigh-Ritz type projection, i.e., multiplying (11) with a Y_j^T, e.g., $Y_j = U_j$, and solving the resulting small $q \times q$ generalized eigenvalue problem

$$Y_j^T (A_j U_j - T_j) E = (Y_j^T U_j) E \Lambda \ . \tag{13}$$

Since the problems (10) and (11) have the same form, the problem (11) can be further transferred in the same FAS way to other levels and to obtain (E, Λ) on the last level, e.g., on the coarsest level. The process of obtaining (E, Λ) by transferring the eigenvalue problem to other levels is called the MG projection (MGP). The MGP is a MG generalization of the Rayleigh-Ritz projection [20,6].

Backrotations [6] are techniques introduced for preventing rotations of solutions in subspaces of eigenvectors with equal or close eigenvalues, and for preventing permutations, rescalings, and sign changing of solutions during processing. In the presented algorithm, the backrotations are used after the computation of (E, Λ) by a MGP, since E may permute or mix the eigenvectors. Permutations and mixing appear especially in degenerate eigenspaces. If degenerate subspaces are present, the

backrotation should bring E to a form close to block diagonal and having on diagonal blocks close to the identity matrix. This is achieved by sorting the eigenvalues in Λ, permuting correspondingly the columns of E, and multiplying E by a block diagonal matrix, having on diagonal the inverses of the E's diagonal blocks associated to equal eigenvalues, followed by rescaling of columns.

III. MG TECHNIQUES FOR THE TREATMENT OF THE NONLINEARITY

The central techniques for nonlinear problems are illustrated on the nonlinear Schrödinger Poisson EP (1). The treatment of the nonlinearity is performed by updating the nonlinear potential W simultaneously with the eigenvectors as well as with the global constraints. The following MG techniques are presented: a MG-potential-solver cycle for W, a simultaneous-FAS cycle for W and eigenvectors, the treatment of the global constraints, the subspace continuation procedures, and the simultaneous-nonlinear-FMG algorithm.

A. A MG solver cycle for the nonlinear potential

In a MG cycle for updating W, we have two options: (1) to keep the u^i's fixed and (2) to update also the u^i's. The first case leads to sequential cycles where separate cycles are performed for W and for u. The second case leads to simultaneous cycles. The two cases lead to different FAS transfers. In this section the u^i's are considered fixed, while in Sec. III B the u^is are updated together with W. The equation to be solved for the nonlinear potential W is

$$\Delta_k W_k = p_k \ . \tag{14}$$

Here, for $k < m$, p_k is the FAS right hand side of (14),

$$p_k = I^k_{k+1}(p_{k+1} - \Delta_{k+1} W_{k+1}) + \Delta_k I^k_{k+1} W_{k+1} \ . \tag{15}$$

On the finest level, $k = m$,

$$p_k = -c_1 \sum_{i=1}^{q} (u^i_k)^2 + c_2 \ . \tag{16}$$

A MG-potential-solver cycle for W is

$(W_m) \leftarrow$ **MG-Potential-Solver** (m, W_m, p_m, l)
For $k = m, \ldots, l$ **(step by** -1**) do:**
$W_k \leftarrow$**Relax** (m, W_k, p_k, k, l)
If $k > l$ **Transfer:**
$W_{k-1} = I^{k-1}_k W_k$,
$p_{k-1} = I^{k-1}_k (p_k - \Delta_k W_k) + \Delta_{k-1} W_{k-1}$
End
For $k = l, \ldots, m$ **(step by 1) do:**
If $(k > l)$ **Correct**
$W_k = W_k + I^k_{k-1}(W_{k-1} - I^{k-1}_k W_k)$
$W_k \leftarrow$**Relax** (m, W_k, p_k, k, l)
End

This is the usual V type cycle from fine level m to coarse level l. Other cycles can be defined as well which involve a different sequence of visiting the levels. The work involved by such a cycle is several times (about four times) the finest level relaxation work. Such a cycle can be used in the next algorithms instead relaxations for W, but in the numerical tests this was not necessary. Similar solver cycles can be defined for the u^i.

B. The MG simultaneous updating of nonlinear potential and eigenvectors

In the MG potential solver, the u_i's are fixed. A MG simultaneous-FAS cycle is obtained by combining the updating of u^is with the updating of W. The nonlinear equations in FAS form are

$$\Delta_k u^i_k - (V_k + \epsilon W_k) u^i_k - \lambda_i u^i_k = \tau^i_k \ , \tag{17}$$

$$\Delta_k W_k + c_1 \sum_{i=1}^{q} (u^i_k)^2 - c_2 = p_k \ . \tag{18}$$

Denote by L_k the operator

$$L_k = \Delta_k - V_k - \epsilon W_k - \lambda_i \ . \tag{19}$$

Both W_k and u_k are considered variables. The τ^i_k and p_k, in (17) and (18), are zero on the finest level and equal to the FAS right hand sides on the other levels, namely,

$$\tau^i_k = I^k_{k+1}(\tau^i_{k+1} - L_{k+1} u^i_{k+1}) + L_k I^k_{k+1} u^i_{k+1} \ , \tag{20}$$

$$p_k = I^k_{k+1} \left(p_{k+1} - \Delta_{k+1} W_{k+1} - c_1 \sum_{i=1}^{q} (u^i_{k+1})^2 \right) + \Delta_k I^k_{k+1} W_{k+1} + c_1 \sum_{i=1}^{q} (I^k_{k+1} u^i_{k+1})^2 \ . \tag{21}$$

The u^i_k's are updated by relaxations, using (17) while W_k is considered constant. W_k is updated by relaxations using (18) while $u^1_k, \ldots, u^q_k$ are considered constants. The u^i_k's are updated by projections and backrotations on coarse levels. The simultaneous-FAS cycle in Sec. III E describes this algorithm.

C. The MG treatment of global constraints

The FAS treatment of global constraints is needed to keep the approximate solutions in the appropriate neighborhood of the exact solutions, where the algorithm is efficient. Keeping the solutions in an appropriate neighborhood is accomplished in conjunction with the simultaneous techniques, the subspace continuation techniques, and the FMG algorithm. The solutions should satisfy several global constraints. The parameter c_1 is set arbitrarily to $c_1 = 1$ but it can also be used as a parameter in a continuation technique. The potential V is periodic and the solutions u_k^i are periodic. Thus W is periodic; therefore

$$\int \Delta W = 0 \ . \tag{22}$$

The integral is taken over the whole domain. Discretizing (22) and using (18), c_2 must satisfy on the current finest grid

$$c_2 = \sum_{j=1}^{N_m} \sum_{i=1}^{q} (u_{m,j}^i)^2 / N_m \ , \tag{23}$$

where N_m is the number of nodes on grid m. Since on the current finest level

$$\|u_m^i\| = 1 \ , \tag{24}$$

c_2 results independent of u and it is kept constant on all levels.

If W is a solution then for any constant C, $W+C$ is also a solution for the same eigenvectors and the eigenvalues $\lambda_i - C$. The constant C is fixed by the condition on W:

$$\int W = 0 \ . \tag{25}$$

The FAS formulation of the discretized condition (25) is

$$\sum_{j=1}^{N_m} W_m^j = 0 \tag{26}$$

on all levels, if the fine to coarse grid transfers conserve zero sums, e.g., as the full weighting transfer which is often used. Otherwise the appropriate FAS condition should be set using (5).

The FAS formulation of the norm condition $\|u_k\| = 1$ becomes [for $Fu = \|u\|$ in (3); see also [2]]

$$\|u_{k-1}\| = \rho_{k-1} := \|I_k^{k-1} u_k\| + \rho_k - \|u_k\| \ . \tag{27}$$

The norms are set to 1 after interpolating the solution the first time to the current finest level and are set to the ρ_k values, on the coarsest levels, at the end of the backrotations. In (27) the same norm notation has been used for the different norms on the different levels.

D. MG subspace continuation techniques

The central idea of subspace-continuation techniques is to use a stable subspace of solutions of a given eigenvalue problem to approximate the subspace of solutions of the problem perturbed. It is important that the subspace of the perturbed problem is well approximated and not the solutions of the perturbed problem. The solutions inside the stable subspace may be very sensitive to perturbations. Subspace-continuation procedures can depend on one, on several, or on a continuum of parameters, e.g., the continuation can be performed by the parameter μ varied from 0 to 1 for μW; or by two parameters α, μ for $\alpha V + \mu W$; or the parameters may be the elements of W.

The continuation process on the coarsest level which we used most in our tests is the following. First the linear problem is solved by a sequence of relaxations, orthogonalizations, and projections for $W = 0$ fixed. This is to approximate first the subspace of the eigenvectors and not the eigenvectors themselves. Then the problem with the potential

$$V_1 = V + \mu W \tag{28}$$

is considered, where μ is a parameter. In the continuation procedure, the μ increases in steps, from 0 to ϵ. At each step, the linear problem is resolved, considering W fixed, and afterwards W is recomputed. Thus the subspace is updated first. This would mean performing the continuation on μW. A continuation using two parameters is to solve first the linear problem for $V = 0$, then perform a continuation on μW until $\mu = \epsilon$ is reached, and only after that to start a continuation process on the linear part of the potential αV. The justification to do this comes from the fact that V may split degenerate eigenspaces in clusters with very close eigenvalues. The continuation having all elements of W as parameters consists in self-consistent iterations in which the linear problem is solved in turns with the updating of W.

The single level continuation procedures described above can be performed in a MG way, leading to MG sequential self-consistent schemes. See also [14] for a MG sequential self-consistent scheme. A more general MG sequential self-consistent scheme is the following MG sequential-continuation algorithm, which iterates the simultaneous updating of the eigenvectors by MG cycles with the updating of W by MG cycles.

$(U_m, W_m, \Lambda) \leftarrow$ **MG-Sequential-Continuation**(U_m, W_m, Λ)
Set $\mu = 0$
While $0 \leq \mu \leq \epsilon$ **do :**
solve until convergence:
1) Solve the linear problem for fixed W_m and potential $V_m + \mu W_m$
$(U_m, \Lambda, \tau_m) \leftarrow$ **U-Simultaneous-FAS**$(m, q, U_m, W_m, \Lambda, L_m, \tau_m, \nu_1, \nu_2)$
2) Solve for W_m keeping U_m, Λ fixed:
$(W_m) \leftarrow$ **MG-Potential-Solver** (m, W_m, p_m, l)
Update W_m such that: $\sum_{j=1}^{N_m} W_m^j = 0$
Increase μ

The above U-simultaneous-FAS algorithm is obtained by removing from the simultaneous-FAS algorithm presented in Sec. III E the updating of W, p, ρ. This is an algorithm for simultaneously updating the eigenvectors, which separates the eigenvectors by projection on a coarse level. The different MG cycles for the eigenvectors and potential may have different coarsest levels. The MG-sequential-continuation procedure can be used on coarse levels at initial stages. Such a procedure may be expensive on fine levels, numerical tests showing that on fine levels often a large number of iterations are necessary for convergence, or that the procedure may even not converge. An efficient alternative is the simultaneous-nonlinear-FMG procedure presented next.

E. The simultaneous nonlinear FMG eigenvalue algorithm

The FMG algorithm for the nonlinear Schrödinger-Poisson EP is presented next. Assume for simplicity, in this section, that on the coarsest level $k = 1$ all eigenvectors can be well approximated. Denote by $U_k = (u_k^1, ..., u_k^q)$ the matrix on level k having as columns the approximations of the desired q eigenvectors, corresponding to the eigenvalues of $\Lambda = \mathrm{diag}(\lambda_1, ..., \lambda_q)$. Assume the same type of vector notations for τ_k, p_k, and ρ_k. The simultaneous-nonlinear-FMG algorithm for q eigenvectors, m levels, reads as follows.

Simultaneous-Nonlinear-FMG$(m, q, U_m, W_m, \Lambda, L_m, \tau_m, \rho_m, p_m, \nu_1, \nu_2, \gamma)$
Set U_1 **random,** $\Lambda = 0, W_1 = 0$
For $k = 1$ **until** m **do:**
1) **If** $k = 1$ get:
$(U_k, W_k, \Lambda) \leftarrow$ **Continuation**(U_k, W_k, Λ)
If $k < m$ **then:** $k = k + 1$
2) Interpolate
$U_k = I_{k-1}^k U_{k-1}$,
$W_k = I_{k-1}^k W_{k-1}$
3) **Set** $\tau_k = 0, \quad \rho_k = 1, \quad c_2 = \sum_{j=1}^{N_k} \sum_{i=1}^{q} (u_{k,j}^i)^2 / N_k, \quad p_k = 0$
$\|u_k^i\| = 1$, $\lambda_i = \langle (\Delta_k - V_k - \epsilon W_k) u_k^i, u_k^i \rangle$
4) **Do** γ **times :**
$(U_k, W_k, \Lambda) \leftarrow$ **Simultaneous-FAS**$(k, q, U_k, W_k, \Lambda, L_k, \tau_k, \rho_k, p_k, \nu_1, \nu_2)$
Endif

Continuation(U_k, W_k, Λ)
Set $\mu = 0$
While $0 \leq \mu \leq \epsilon$ **do :**
If $\mu = 0$ get U_k, Λ by Relaxations, Orthogonalizations and Projections
Else solve until convergence steps 1, 2:
1) Solve the linear problem for U_k, Λ by Relaxations and Projections.
2) Solve for W_k : $\Delta_k W_k + c_1 \sum_{i=1}^{q} (u_k^i)^2 = c_2, \quad \sum_{j=1}^{N_k} W_k^j = 0$
Endif
Increase μ

Simultaneous-FAS$(k, q, U_k, W_k, \Lambda, L_k, \tau_k, \rho_k, p_k, \nu_1, \nu_2)$
For $k = m, \ldots, 1$ **step** -1 **do:**
If $k = 1$ **do:**
1) $(U_k, W_k, \Lambda) \leftarrow$ **CoarseLevel**$(k, q, L_k, U_k, W_k, \Lambda, \tau_k, \rho_k, p_k)$
Else
2) Relax ν_1 times with initial guess U_k, W_k :

TABLE I. The residuals and eigenvalues of the first five eigenvectors of the discretized nonlinear Schrödinger-Poisson EP in 2D, on six levels, computed by a 1-FMG-V(1,1) simultaneous algorithm. On the first level five cycles were performed and on the second level three cycles. The projection was performed on level 2. Seven cycles were performed on the finest level to illustrate a constant convergence rate per MG cycle of 0.15. The residuals are computed at the start and at the end of the $V(1,1)$ cycles; and the eigenvalues at the end of the cycles by Rayleigh quotients. The decrease of the residuals by a factor of 4 from one level to the next (the start residuals in the first cycle, on fine levels) indicates a second order convergence towards the differential solution for the eigenvectors.

Cycle	Vector	Start res.	End res.	Eigenvalue
		Level 1		
5	1	0.37×10^{-13}	0.46×10^{-13}	$-0.15528834591395\times10^{2}$
	2	0.12×10^{-12}	0.84×10^{-13}	$-0.90047054014218\times10^{2}$
	3	0.85×10^{-13}	0.79×10^{-13}	$-0.90047054014218\times10^{2}$
	4	0.74×10^{-12}	0.26×10^{-12}	$-0.10369602966161\times10^{3}$
	5	0.12×10^{-11}	0.45×10^{-12}	$-0.10369602966161\times10^{3}$
		Level 2		
1	1	0.44×10^{1}	0.50×10^{-3}	$-0.15182335042395\times10^{2}$
	2	0.30×10^{2}	0.22×10^{-1}	$-0.10144043667188\times10^{3}$
	3	0.30×10^{2}	0.22×10^{-1}	$-0.10144043667188\times10^{3}$
	4	0.32×10^{2}	0.47×10^{-1}	$-0.12014770030904\times10^{3}$
	5	0.32×10^{2}	0.47×10^{-1}	$-0.12014770030904\times10^{3}$
3	1	0.17×10^{-5}	0.60×10^{-8}	$-0.15182335072480\times10^{2}$
	2	0.43×10^{-4}	0.88×10^{-7}	$-0.10144043560798\times10^{3}$
	3	0.43×10^{-4}	0.88×10^{-7}	$-0.10144043560798\times10^{3}$
	4	0.19×10^{-3}	0.84×10^{-6}	$-0.12014769418108\times10^{3}$
	5	0.19×10^{-3}	0.84×10^{-6}	$-0.12014769418108\times10^{3}$
		Level 3		
1	1	0.13×10^{1}	0.59×10^{-1}	$-0.15069813064192\times10^{2}$
	2	0.11×10^{2}	0.46×10^{-1}	$-0.10444903871181\times10^{3}$
	3	0.11×10^{2}	0.46×10^{-1}	$-0.10444903871181\times10^{3}$
	4	0.12×10^{2}	0.88×10^{-1}	$-0.12465344903258\times10^{3}$
	5	0.12×10^{2}	0.88×10^{-1}	$-0.12465344903258\times10^{3}$
		Level 4		
1	1	0.36×10^{0}	0.22×10^{-1}	$-0.15039575054851\times10^{2}$
	2	0.31×10^{1}	0.32×10^{-1}	$-0.10521096070648\times10^{3}$
	3	0.31×10^{1}	0.32×10^{-1}	$-0.10521096070648\times10^{3}$
	4	0.33×10^{1}	0.19×10^{-1}	$-0.12580555034765\times10^{3}$
	5	0.33×10^{1}	0.19×10^{-1}	$-0.12580555034763\times10^{3}$
		Level 5		
1	1	0.95×10^{-1}	0.65×10^{-2}	$-0.15031924453065\times10^{2}$
	2	0.79×10^{0}	0.13×10^{-1}	$-0.10540212079295\times10^{3}$
	3	0.79×10^{0}	0.13×10^{-1}	$-0.10540212079291\times10^{3}$
	4	0.85×10^{0}	0.85×10^{-2}	$-0.12609530927232\times10^{3}$
	5	0.85×10^{0}	0.85×10^{-2}	$-0.12609530927231\times10^{3}$
		Level 6		
1	1	0.24×10^{-1}	0.17×10^{-2}	$-0.15030004902969\times10^{2}$
	2	0.20×10^{0}	0.39×10^{-2}	$-0.10544995104364\times10^{3}$
	3	0.20×10^{0}	0.39×10^{-2}	$-0.10544995104306\times10^{3}$
	4	0.21×10^{0}	0.28×10^{-2}	$-0.12616785302342\times10^{3}$
	5	0.21×10^{0}	0.28×10^{-2}	$-0.12616785302487\times10^{3}$
3	1	0.17×10^{-3}	0.18×10^{-4}	$-0.15030004885985\times10^{2}$
	2	0.46×10^{-3}	0.55×10^{-4}	$-0.10544995101300\times10^{3}$
	3	0.46×10^{-3}	0.55×10^{-4}	$-0.10544995101134\times10^{3}$
	4	0.34×10^{-3}	0.42×10^{-4}	$-0.12616785302509\times10^{3}$
	5	0.34×10^{-3}	0.42×10^{-4}	$-0.12616785302485\times10^{3}$
7	1	0.29×10^{-7}	0.88×10^{-8}	$-0.15030004896583\times10^{2}$
	2	0.92×10^{-7}	0.11×10^{-7}	$-0.10544995101183\times10^{3}$
	3	0.92×10^{-7}	0.11×10^{-7}	$-0.10544995101118\times10^{3}$
	4	0.80×10^{-7}	0.11×10^{-7}	$-0.12616785302732\times10^{3}$
	5	0.80×10^{-7}	0.99×10^{-8}	$-0.12616785302532\times10^{3}$

$\Delta_k W_k + c_1 \sum_{i=1}^{q} (u_k^i)^2 - c_2 = p_k, \quad \sum_{j=1}^{N_k} W_k^j = 0$
$L_k U_k = \tau_k$
3) Compute the residual $r_k = \tau_k - L_k U_k$
4) Restrict $\tau_{k-1} = L_{k-1} I_k^{k-1} U_k + I_k^{k-1} r_k$
5) Set $p_{k-1} = \Delta_{k-1} I_k^{k-1} W_k + \sum_{i=1}^{q} (I_k^{k-1} u_k^i)^2 + I_k^{k-1}(p_k - \Delta_k W_k - \sum_{i=1}^{q} (u_k^i)^2)$
6) Set $\rho_{k-1} = \| I_k^{k-1} U_k \| + \rho_k - \| U_k \|$
7) Restrict :
$U_{k-1} = I_k^{k-1} U_k,$
$W_{k-1} = I_k^{k-1} W_k$

Endif

For $k = 2, \ldots, m$ **step** 1 **do:**
9) **If** $k < m$ Interpolate and FAS correct:
$U_k = U_k + I_{k-1}^k (U_{k-1} - I_k^{k-1} U_k)$
$W_k = W_k + I_{k-1}^k (W_{k-1} - I_k^{k-1} W_k)$

Endif
10) Relax ν_2 times:
$L_k U_k = \tau_k$
$\Delta_k W_k + c_1 \sum_{i=1}^{q} (u_k^i)^2 - c_2 = p_k, \quad \sum_{j=1}^{N_k} W_k^j = 0$

CoarseLevel$(k, q, L_k, U_k, W_k, \Lambda, \tau_k, \rho_k, p_k)$
Do until convergence :
1) Update (U_k, Λ) by Projection and Backrotation
2) Solve for W:
$\Delta_k W_k + c_1 \sum_{i=1}^{q} (u_k^i)^2 - c_2 = p_k, \quad \sum_{j=1}^{N_k} W_k^j = 0$
3) Relax $L_k U_k = \tau_k$

In the simultaneous-nonlinear-FMG algorithm, at step 3, the eigenvalues are updated by Rayleigh quotients: $\lambda_i = \langle (\Delta_k - V_k - \epsilon W_k) u_k^i, u_k^i \rangle / \langle u_k^i, u_k^i \rangle$. The constant γ is the number of cycles performed on each level. ν_1, (ν_2) is the number of relaxations performed in the simultaneous cycle, on each level in the path from fine to coarse (coarse to fine). Such a V cycle will be denoted $V(\nu_1, \nu_2)$ and the FMG with γ cycles as above will be denoted by γ-FMG-$V(\nu_1, \nu_2)$.

If not all desired eigenvectors can be well approximated on coarsest level then the nonlinear-FMG algorithm can be used in an adaptive version in which the nonlinear FMG is performed for clusters of close or equal eigenvalues, each cluster having its own coarsest level. The single difference is that in the computations of p the sums for the eigenvectors are performed not only for the eigenvectors in the cluster but for all eigenvectors in the other approximated clusters, on the common levels (else a restriction of W can be used). The clusters of close and equal eigenvalues have to be completed in order to obtain robustness and efficiency. The constants γ, ν_1, and ν_2 and the coarse level on which to perform the projection efficiently can be found adaptively. For this the adaptive techniques presented in [6] can be used.

F. Storage, work, and accuracy

In the algorithm presented in the previous section, storage is required for the q eigenvectors u_k^i of size N on the finest grid, the potentials, and the corresponding right hand sides, on all levels, giving an overall estimate of memory of order $O(3(N+3))$ for problems in 2D and

TABLE II. The residuals of the nonlinear potential W of the discretized nonlinear Schrödinger-Poisson EP in 2D, on six levels, computed by a 1-FMG-V(1,1) simultaneous algorithm. Three relaxations were performed for W. On the first level five cycles were performed and on the second level three cycles. Seven cycles were performed on the finest level to illustrate a constant convergence rate per MG cycle of 0.15. The residuals are computed at the start and at the end of the MG cycles. The decrease of the residuals by a factor of 4 from one level to the next (the start residuals in the first cycle, on fine levels) indicates a second order convergence towards the differential solution for W.

Cycle	Start res.	End res.
	Level 1	
1	0.11×10^{-9}	0.10×10^{-13}
	Level 2	
1	0.35×10^{0}	0.16×10^{-3}
2	0.16×10^{-3}	0.59×10^{-6}
3	0.59×10^{-6}	0.23×10^{-8}
	Level 3	
1	0.36×10^{-1}	0.13×10^{-3}
	Level 4	
1	0.69×10^{-2}	0.11×10^{-3}
	Level 5	
1	0.17×10^{-2}	0.37×10^{-4}
	Level 6	
1	0.44×10^{-3}	0.11×10^{-4}
2	0.11×10^{-4}	0.86×10^{-6}
3	0.86×10^{-6}	0.98×10^{-7}
4	0.98×10^{-7}	0.12×10^{-7}
5	0.12×10^{-7}	0.14×10^{-8}
6	0.14×10^{-8}	0.16×10^{-9}
7	0.16×10^{-9}	0.21×10^{-10}

3D. The work requires $O(N)$ operations per eigenvector and $O(N)$ operations for the nonlinear potential. The work performed on the coarsest grids should be added to these estimates. Usually this work does not change the complexity of the algorithm, being only a part of the fine level work. In the case of degenerate or clustered eigenvalues, if scalar products accurately 0 are needed on the finest levels, inside the degenerate or clustered eigenspaces, then orthonormalizations may be required within these eigenspaces on the finest level. However, as can be seen in the computational examples, accurate orthogonality inside degenerate clusters may be obtained by coarse level separation also. The schemes presented $O(h^2)$ accuracy for the five-point in 2D and nine-point in 3D Laplacians, for a 1-FMG-V(1,1) algorithm, as seen in the outputs, where h is the step size.

IV. COMPUTATIONAL RESULTS

Computational results of the algorithm presented in Sec. III E are presented and discussed further. Tables I and II present results for the 2D, nonlinear eigenvalue problem (1) with the potential $V(x,y) = 14 - (2\pi/a)^2 f(x,y)/[7 + f(x,y)]$. Here $f(x,y) = \sin(10x + 10y) + \cos(10x + 10y)$ ($a = 2\pi/10$ is the size of the domain

TABLE III. The residuals and eigenvalues of the first seven eigenvectors of the discretized nonlinear Schrödinger-Poisson EP in 3D, on three levels, computed by a 4-FMG-V(1,1) simultaneous algorithm. The linear potential is $V(x,y,z) = 14 - 100\sin(10x+10y+10z)/[30+\sin(10x+10y+10z)]$. On the first level seven cycles were performed. The projection was performed on level 2. The residuals are computed at the start and at the end of the $V(1,1)$ cycles; and the eigenvalues at the end of the cycles. Observe the six equal eigenvalues.

Cycle	Vector	Start res.	End res.	Eigenvalue
		Level 1		
7	1	0.89×10^{-13}	0.76×10^{-13}	$-0.14048591304840\times10^{2}$
	2	0.93×10^{-9}	0.38×10^{-9}	$-0.95098529109559\times10^{2}$
	3	0.93×10^{-9}	0.38×10^{-9}	$-0.95098529109559\times10^{2}$
	4	0.93×10^{-9}	0.38×10^{-9}	$-0.95098529109559\times10^{2}$
	5	0.93×10^{-9}	0.38×10^{-9}	$-0.95098529109559\times10^{2}$
	6	0.93×10^{-9}	0.38×10^{-9}	$-0.95098529109559\times10^{2}$
	7	0.93×10^{-9}	0.38×10^{-9}	$-0.95098529109559\times10^{2}$
		Level 2		
1	1	0.90×10^{0}	0.33×10^{-2}	$-0.14040128427761\times10^{2}$
	2	0.30×10^{2}	0.18×10^{0}	$-0.10899132948707\times10^{3}$
	3	0.30×10^{2}	0.18×10^{0}	$-0.10899132948707\times10^{3}$
	4	0.30×10^{2}	0.18×10^{0}	$-0.10899132948707\times10^{3}$
	5	0.30×10^{2}	0.18×10^{0}	$-0.10899132948707\times10^{3}$
	6	0.30×10^{2}	0.18×10^{0}	$-0.10899132948707\times10^{3}$
	7	0.30×10^{2}	0.18×10^{0}	$-0.10899132948707\times10^{3}$
4	1	0.22×10^{-7}	0.17×10^{-8}	$-0.14040128424469\times10^{2}$
	2	0.30×10^{-3}	0.23×10^{-4}	$-0.10899126009610\times10^{3}$
	3	0.30×10^{-3}	0.23×10^{-4}	$-0.10899126009610\times10^{3}$
	4	0.30×10^{-3}	0.23×10^{-4}	$-0.10899126009610\times10^{3}$
	5	0.30×10^{-3}	0.23×10^{-4}	$-0.10899126009610\times10^{3}$
	6	0.30×10^{-3}	0.23×10^{-4}	$-0.10899126009610\times10^{3}$
	7	0.30×10^{-3}	0.23×10^{-4}	$-0.10899126009610\times10^{3}$
		Level 3		
1	1	0.25×10^{0}	0.46×10^{-1}	$-0.14036829480230\times10^{2}$
	2	0.11×10^{2}	0.69×10^{0}	$-0.11274758485900\times10^{3}$
	3	0.11×10^{2}	0.69×10^{0}	$-0.11274758485900\times10^{3}$
	4	0.11×10^{2}	0.69×10^{0}	$-0.11274758485900\times10^{3}$
	5	0.11×10^{2}	0.69×10^{0}	$-0.11274758485900\times10^{3}$
	6	0.11×10^{2}	0.69×10^{0}	$-0.11274758485900\times10^{3}$
	7	0.11×10^{2}	0.69×10^{0}	$-0.11274758485900\times10^{3}$
4	1	0.58×10^{-3}	0.65×10^{-4}	$-0.14036815617277\times10^{2}$
	2	0.20×10^{-2}	0.30×10^{-3}	$-0.11274310146319\times10^{3}$
	3	0.20×10^{-2}	0.30×10^{-3}	$-0.11274310146319\times10^{3}$
	4	0.20×10^{-2}	0.30×10^{-3}	$-0.11274310146319\times10^{3}$
	5	0.20×10^{-2}	0.30×10^{-3}	$-0.11274310146319\times10^{3}$
	6	0.20×10^{-2}	0.30×10^{-3}	$-0.11274310146319\times10^{3}$
	7	0.20×10^{-2}	0.30×10^{-3}	$-0.11274310146319\times10^{3}$

in both directions). V is chosen so in order to determine a cluster consisting of two clusters of two equal eigenvalues. A 1-FMG-V(1,1) algorithm was used to show that one $V(1,1)$ cycle per level is enough to obtain a second order convergence towards the continuous solution. See for this the residuals at the start of the first V cycle on each level decreasing by a factor of about 4 from one level to the next finer level. (The mesh size decreases by a factor of 2 from one level to the next finer one.) Seven V cycles were performed on finest level 6, to show the convergence rate for eigenvectors and potential, better than 0.15 in all cycles. The convergence rate is the same for all eigenvectors in the cluster, of order 0.15 in all cycles from 3 to 7. For the potential W, three relaxations were used, but a MG cycle for W could be employed as well instead (this was not needed in the tests performed). The separation by projection is performed on level 2 instead of 1 and the eigenvalue systems were solved exactly on the coarsest level. The eigenvectors are normalized to 1 on the finest level. The presented eigenvalues are computed by Rayleigh quotients on the finest levels. (Generally, the fine level Rayleigh quotients are not necessary, the coarse level projection providing accurate eigenvalues, but they have been shown to improve the efficiency of at least the

TABLE IV. The residuals and eigenvalues of the first seven eigenvectors of the discretized nonlinear Schrödinger-Poisson EP in 3D, on three levels, computed by a 4-FMG-V(1,1) simultaneous algorithm. The linear potential is $V(x,y,z) = 14-100\sin(30x+20y+10z)/[30+\sin(30x+20y+10z)]$. On the first level seven cycles were performed. The projection was performed on level 2. The residuals are computed at the start and at the end of the $V(1,1)$ cycles; and the eigenvalues at the end of the cycles. Observe the six eigenvalues with six common digits in the cluster of six consisting in three degenerate clusters.

Cycle	Vector	Start res.	End res.	Eigenvalue
		Level 1		
7	1	0.52×10^{-12}	0.23×10^{-12}	$-0.14055580293076\times10^{2}$
	2	0.19×10^{-7}	0.11×10^{-7}	$-0.95112505605267\times10^{2}$
	3	0.23×10^{-7}	0.59×10^{-8}	$-0.95112505605267\times10^{2}$
	4	0.47×10^{-8}	0.14×10^{-7}	$-0.95112516406102\times10^{2}$
	5	0.44×10^{-7}	0.12×10^{-7}	$-0.95112516406102\times10^{2}$
	6	0.43×10^{-8}	0.75×10^{-9}	$-0.95112516406102\times10^{2}$
	7	0.54×10^{-8}	0.64×10^{-9}	$-0.95112516406102\times10^{2}$
		Level 2		
1	1	0.13×10^{1}	0.13×10^{-4}	$-0.14053758492811\times10^{2}$
	2	0.30×10^{2}	0.17×10^{0}	$-0.10901746968777\times10^{3}$
	3	0.30×10^{2}	0.17×10^{0}	$-0.10901746968777\times10^{3}$
	4	0.30×10^{2}	0.17×10^{0}	$-0.10901758164786\times10^{3}$
	5	0.30×10^{2}	0.17×10^{0}	$-0.10901758164786\times10^{3}$
	6	0.30×10^{2}	0.17×10^{0}	$-0.10901781869743\times10^{3}$
	7	0.30×10^{2}	0.17×10^{0}	$-0.10901781869743\times10^{3}$
4	1	0.35×10^{-10}	0.12×10^{-10}	$-0.14053758492812\times10^{2}$
	2	0.38×10^{-5}	0.21×10^{-7}	$-0.10901741800157\times10^{3}$
	3	0.38×10^{-5}	0.21×10^{-7}	$-0.10901741800157\times10^{3}$
	4	0.17×10^{-4}	0.83×10^{-6}	$-0.10901752982146\times10^{3}$
	5	0.17×10^{-4}	0.83×10^{-6}	$-0.10901752982146\times10^{3}$
	6	0.37×10^{-5}	0.17×10^{-7}	$-0.10901776702773\times10^{3}$
	7	0.37×10^{-5}	0.17×10^{-7}	$-0.10901776702773\times10^{3}$
		Level 3		
1	1	0.13×10^{1}	0.25×10^{0}	$-0.14051499340829\times10^{2}$
	2	0.11×10^{2}	0.75×10^{0}	$-0.11277655294003\times10^{3}$
	3	0.11×10^{2}	0.75×10^{0}	$-0.11277655294003\times10^{3}$
	4	0.11×10^{2}	0.75×10^{0}	$-0.11277700995289\times10^{3}$
	5	0.11×10^{2}	0.75×10^{0}	$-0.11277700995289\times10^{3}$
	6	0.11×10^{2}	0.74×10^{0}	$-0.11277731911554\times10^{3}$
	7	0.11×10^{2}	0.74×10^{0}	$-0.11277731911554\times10^{3}$
4	1	0.29×10^{-2}	0.32×10^{-3}	$-0.14051251375940\times10^{2}$
	2	0.64×10^{-2}	0.96×10^{-3}	$-0.11277176295116\times10^{3}$
	3	0.64×10^{-2}	0.96×10^{-3}	$-0.11277176295116\times10^{3}$
	4	0.92×10^{-2}	0.17×10^{-2}	$-0.11277225319175\times10^{3}$
	5	0.92×10^{-2}	0.17×10^{-2}	$-0.11277225319175\times10^{3}$
	6	0.55×10^{-2}	0.80×10^{-3}	$-0.11277260890858\times10^{3}$
	7	0.55×10^{-2}	0.80×10^{-3}	$-0.11277260890858\times10^{3}$

TABLE V. The residuals of the nonlinear potential W of the discretized nonlinear Schrödinger-Poisson EP in 3D, on three levels, computed by a 4-FMG-V(1,1) simultaneous algorithm. Three relaxations were performed for W. The residuals are computed at the start and at the end of the MG cycles.

Cycle	Start res.	End res.
	Level 1	
7	0.49×10^{-10}	0.20×10^{-10}
	Level 2	
1	0.38×10^{0}	0.13×10^{-4}
2	0.13×10^{-4}	0.72×10^{-7}
3	0.72×10^{-7}	0.20×10^{-8}
4	0.20×10^{-8}	0.99×10^{-10}
	Level 3	
1	0.30×10^{-1}	0.39×10^{-3}
2	0.39×10^{-3}	0.52×10^{-4}
3	0.52×10^{-4}	0.72×10^{-5}
4	0.72×10^{-5}	0.10×10^{-5}

first cycle on each level. In the first cycle, the eigenvalues are improved by the quotients and used on the path down before they are recomputed by the projection. This first cycle is generally sufficiently efficient for obtaining a second order scheme so that additional cycles are not necessary, at least until the finest level where one may desire accurate converged solutions, and thus would employ several more cycles.) The degenerate eigenvalues come out with 11–14 equal digits. The convergence rate of the nonlinear potential is also about 0.15 per cycle, as for the eigenvectors; see Table II. Accurate separation is obtained in the cluster and in degenerate eigenspaces, although the separation was performed on the coarse level 2. The scalar products on level 6 are of order 10^{-12} [15]. Although the clusters are well separated, a relatively strong mixing of solutions appears especially on coarse levels motivating the MGP.

Tables III–IV present results for problems in 3D which are similar to the 2D results. The first seven eigenvectors were sought. The problems were discretized on three levels. The cycles were $V(1,1)$ and the projections were performed on the second level.

The potential $V(x,y,z) = 14 - 100\sin(10x + 10y + 10z)/[30 + \sin(10x + 10y + 10z)]$ provides a cluster of six degenerate eigenvalues, presented in Table III. The approximations of the degenerate eigenvalues present 13 equal digits, on levels 2 and 3. The results in Table IV are for the same problem with nonsymmetric V, $V(x,y,z) = 14 - 100\sin(30x + 20y + 10z)/[30 + \sin(30x + 20y + 10z)]$. On the first level, V splits the previous cluster of six eigenvalues into two degenerate clusters of two and four eigenvalues. On levels 2 and 3, the cluster of four degenerate eigenvalues splits into two clusters of two degenerate eigenvalues. The degenerate eigenvalues present 14 equal digits. The six clustered eigenvalues have the first five digits equal. On level 3, the eigenvectors come out exactly orthogonal; their scalar products are of order 10^{-13} [15].

Table V shows the residuals of the nonlinear potential W. The fact that the cluster structure differs on different levels introduces special computational difficulties. The problem has to be defined on complete clusters of eigenvectors and the clusters have to be completed. These difficulties can be detected and treated by the adaptive techniques presented in [6]. The linear potential $V = c + V0$ contains the shift $c = 14$ to obtain a positive V in the relaxations. The eigenvalues for the problem with $V = V0$ are obtained by shifting by 14 the found eigenvalues. The first eigenvalue in the Tables III and IV would become close to 0, i.e., -0.036 and -0.051, showing that without changing the algorithm and by the same computational work the eigenvalues for close to singular or singular operators can be computed.

V. CONCLUSIONS

A MG simultaneous algorithm for the nonlinear Schrödinger-Poisson EP is presented. The algorithm combines the following techniques: the MG projection and backrotations; the MG subspace continuation technique; the FAS treatment of global constraints; the simultaneous processing of eigenvectors, nonlinear potential, and global constraints. In the computational examples, the simultaneous MG technique reduced the large number of sequential self-consistent iterations to one MG simultaneous iteration (1-FMG here). One simultaneous cycle involves fewer computations than one sequential cycle (updating eigenvectors sequentially and separating them on the finest level) due to the cheap coarse level separation by the MGP and backrotations. The MG subspace continuation techniques coupled with the simultaneous processing on all levels helped keep the approximated solution in an appropriate region where the algorithm is efficient. MG projections and backrotations are used to separate the eigenvectors by coarse level work and to overcome difficulties due to close or equal eigenvalues.

Computational examples for the nonlinear Schrödinger-Poisson EP in 2D and 3D having special computational difficulties, which are due to equal and closely clustered eigenvalues, are presented. For these

cases, the algorithm requires $O(qN)$ operations for the calculation of q eigenvectors of size N. The algorithm achieved the same accuracy, using the same amount of work (per eigenvector), as the Poisson MG solver. A second order approximation is obtained using the five-point in 2D and nine-point in 3D discretized Laplacian, by 1-FMG-V(1,1) in $O(qN)$work. The work was of order of a few (about eight) fine level Gauss-Seidel relaxations per eigenvector. Constant convergence rate per cycle of 0.15 was obtained for the presented cases. The numerical tests showed that an accurate fine level separation was obtained by the coarse level projection, even for problems with very close or equal eigenvalues. This reduced the expensive fine level separation work of order $O(q^2N)$ of previous algorithms to coarse level work of order $O(qN)$.

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