Multiscale Eigenbasis Calculations: N Eigenfunctions in $O(N \log N)$

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Abstract. Motivated by quantum chemical calculations, we explore a novel multiscale approach for computing, storing, and expanding in many eigenfunctions of differential operators. This approach leads to efficient multiscale eigenbasis algorithms, which typically scale as $O(N \log N)$, where N is the number of eigenfunctions. In particular, they provide a vast generalization of the Fast Fourier Transform (FFT) algorithm, which expands in Fourier series, to expansions in terms of eigenfunctions of a general 1D linear differential operator with general boundary conditions. Generalizations to higher dimensional eigenproblems are discussed. A complete and detailed discussion of the methods can be found in [14,15].

1 Motivation: Electronic Structure Computations

The basic equations of condensed matter, e.g., the Kohn-Sham equations in ab-initio quantum chemistry [22] have been known for several decades. In principle, one could utilize them for *computerizing chemistry*: controlling chemical interactions and designing materials with prescribed properties (from drugs to missile coating), instead of conducting expensive empirical experiments.

Despite their dazzling speed, even modern supercomputers cannot surmount the highly complicated eigenbasis computations involved. Current numerical eigenbasis algorithms are slow, thus limited to computing moderately complex electronic structures. Linear-complexity algorithms ("$O(N)$ methods") [3,11] have been constructed only under localization assumptions on the electronic orbitals.

Our research goal was to design linear-complexity multiscale algorithms for computing, storing, and manipulating many eigenfunctions of the periodic Schrödinger operator and other related differential operators, *without localization assumptions on the eigenfunctions.*

We have focused mainly on the periodic Schrödinger eigenproblem

$$(-\Delta + V(\boldsymbol{x}))\psi(\boldsymbol{x}) = \lambda\psi(\boldsymbol{x}), \quad \boldsymbol{x} \in \Omega \subset \mathbf{R}^d \,, \tag{1}$$

where $V(x)$ is an Ω-periodic potential function containing $O(N)$ general "features", such as wells representing screened atomic nuclei [20].

Our work has four computational aims:

1. *Computing* and *storing* N distinct eigenfunctions $\psi_j(x)$ and eigenvalues of (1) in $O(N \log N)$ operations;
2. *Integrating (or summing)* N eigenfunctions of (1) into the electronic density function $\varrho(x) = \sum_j |\psi_j(\boldsymbol{x})|^2$ in $O(N \log N)$ operations;
3. *Expanding* a given function in N eigenfunctions of (1) in $O(N \log N)$ operations;
4. *Expanding* a given function in N eigenfunctions of *a general 1D linear differential operator*, in $O(N \log N)$ operations.

The last computational task stems from a natural generalization of the 1D Schrödinger operator to Sturm-Liouville operators and general parameter-dependent ODEs.

1.1 Example: The 1D Linear Case

In actual ab-initio electronic structure computations we encounter the nonlinear (self-consistent) 3D Schrödinger eigenproblem, where V depends on non-local integrals involving the electronic density ϱ [18]. Nevertheless, we chose to start with the 1D linear case ((1) for $d = 1$), because of the following reasons:

- *Isolation of the main obstacle: the multiplicity of eigenfunctions.* Other aspects of the general equations, such as nonlinearity, systems of PDEs, and singularities, have already been treated by multiscale methods in other contexts [4,7].
- *Feasibility.* One cannot hope to construct collective representations of eigenfunctions in 2D and 3D if it cannot be accomplished in 1D. It is true that the 1D implementation includes devices that do not seem to manifest direct higher-dimensional generalizations, most important of which is the concept of monodromy. But indirect generalizations do exist; the monodromy concept can be replaced by coarse-level difference equations (see Sect. 6).
- *Applications to other important 1D problems.* We have generalized our fast expansion and integration algorithms to expansions in eigenfunctions of general linear differential operators and, in particular, to Sturm-Liouville transforms. Although efficient transform procedures already exist for very special cases (such as FFT and FLT – Fast Legendre Transform [15]), our fast transform algorithm is robust and generic, and hence should have broad applications. The 1D Schrödinger eigenproblem itself has important physical applications to 1D conductors and soliton theory [2,16].

2 The Main Complexity Factors

There are three main complexity factors in computing, storing, and manipulating N eigenfunctions of the Schrödinger operator:

1. *Many features in* $V(x)$. The number of spatial points needed for a good resolution of $V(x)$ is $O(N)$; hence each eigenfunction needs at least an $O(N)$-point resolution in x.
2. *Many distinct eigenfunctions.* A large number N of distinct eigenfunctions and eigenvalues need to be computed, representing N electrons.
3. *Many orthogonalization steps.* In order to orthonormalize the eigenbasis, $O(N)$ orthogonalization steps per eigenfunction are needed, each requiring $O(N)$ operations.

Whereas the first two factors result in $O(N^2)$ storage, which is needed to represent $O(N)$ eigenfunctions in the current eigenbasis algorithms (from early algebraic solvers [17] to modern multigrid eigensolvers [9,10]), the third factor raises their complexity to $O(N^3)$.

Our novel approach and methodology is based on the observation that *"neighboring" eigenfunctions (with close "momenta") are distinguishable from each other only at large scales.* Using *collective representations* of eigenfunctions that share the common description of their details at finer scales, and progressively separate them out only on increasingly coarse grids, we have developed algorithms that require only $O(N \log N)$ computer operations and storage, *without localization assumptions on the electronic orbitals* (the theoretical complexity is $O(N(\log N)^2)$ at worst, but it reduces to $O(N \log N)$ in most problems). Even in localized systems, our approach requires only $O(N(\log N_{\text{local}})^2)$ operations in the worst case, versus $O(NN_{\text{local}}^2)$ needed by current localization methods [11], where N_{local} is the number of orbitals in the localized cell.

3 The Main Principle

The 1D collective-eigenfunction approach involves the concept of *monodromy transformation*, which represents the propagation of solutions of

$$\partial_x \boldsymbol{U}(x) = \begin{pmatrix} 0 & 1 \\ V(x) - \lambda & 0 \end{pmatrix} \boldsymbol{U}(x) \,, \qquad \boldsymbol{U}(x) := \begin{pmatrix} \psi(x) \\ \partial_x \psi(x) \end{pmatrix} \,, \tag{2}$$

where $\partial_x = d/dx$. Equation (2) is equivalent to (1) in one dimension.

3.1 The Monodromy Transformation

Equation (2) can be regarded as a parameter-dependent ODE. Hence, every solution $\boldsymbol{U}(x)$ is uniquely determined by its *initial value*, say, at $x = a$.

In other words, the value $\boldsymbol{U}(b)$ depends uniquely on $\boldsymbol{U}(a)$ for any interval $[a,b]$. Since (2) is linear, the transformation $\boldsymbol{U}(a) \longmapsto \boldsymbol{U}(b)$ is a 2×2 matrix $\boldsymbol{M}([a,b];\lambda)$, called the *monodromy matrix* [19]. Some important properties of the monodromy transformation are:

1. *Locality:* the monodromy depends on λ and the values of $V(x)$ inside $[a,b]$ only.
2. *Non-degeneracy:* $\det(\boldsymbol{M}([a,b];\lambda)) = 1$; in particular, $\boldsymbol{M}([a,a];\lambda) = I$.
3. *Multiplicativity:* for every $a < b < c$,

$$\boldsymbol{M}([a,c];\lambda) = \boldsymbol{M}([b,c];\lambda) \cdot \boldsymbol{M}([a,b];\lambda) \; . \tag{3}$$

4. *Relation to boundary value problems:* the function $\boldsymbol{M}(\lambda) := \boldsymbol{M}(\Omega;\lambda)$ and the specific boundary conditions determine the spectrum of (2) [19]. Two examples:
   - Dirichlet B.C.: $\psi(0) = \psi(L) = 0$. Equivalently, the eigenvalues are the roots of the equation

$$\boldsymbol{M}_{12}(\lambda) = 0 \; . \tag{4}$$

   - Quasiperiodic B.C.: given a periodic potential $V(x+L) = V(x)$, $-\infty < x < \infty$, Bloch-type solutions [19]

$$\psi(x+L) = e^{i\beta L}\psi(x), \qquad \beta \in \mathbf{R}, \forall x \in \mathbf{R}$$

     form a *band spectrum* [19]. They represent all the bounded eigenfunctions on the entire space, as required in electronic structure calculations. This spectrum is characterized by the inequality

$$|D(\lambda)| := |\boldsymbol{M}_{11}(\lambda) + \boldsymbol{M}_{22}(\lambda)| \leq 2 \; .$$

3.2 Complementary Smoothness of the Monodromy

The monodromy function $\boldsymbol{M}(I;\lambda)$ of a fixed interval I of length x is an analytic function of λ [19]. Furthermore, its scale of smoothness is inversely proportional to the size of I. For example, in regions where $\lambda - V(x) > 0$, each of its entries is an oscillating function of λ, with a frequency *directly proportional to the length of* I.

This can be easily observed in the special case of $V \equiv 0$, for which

$$\boldsymbol{M}([0,x];\lambda) = \begin{pmatrix} \cos(\omega x) & \omega^{-1}\sin(\omega x) \\ -\omega \sin(\omega x) & \cos(\omega x) \end{pmatrix}, \qquad \omega := \sqrt{\lambda} \; . \tag{5}$$

The frequency of the entries as functions of ω is x. This holds for all nonnegative λs and for the monodromy $\boldsymbol{M}(I;\lambda)$ of *any* interval I of length x, since for a constant potential the monodromy does not depend on the starting point of the spatial interval, but on its length only.

This property of monodromies is called the *complementary smoothness principle*, resembling the *Heisenberg Principle* of quantum mechanics, where x and λ are the complementary dimensions: the *product* of the spatial and eigenvalue resolutions depends *only* on the desired accuracy in the monodromy transformation.

This principle is proved in [14] for monodromies of *any 1D linear differential eigenproblem*. It does not depend on the smoothness of the coefficient functions (such as the potential function $V(x)$). We apply this principle to the construction of efficient multiscale eigenbasis algorithms.

4 The Multiscale Eigenbasis Structure

Our basic tool in fast eigenbasis computations is the Multiscale Eigenbasis (MEB) structure, which implicitly represents $O(N)$ eigenfunctions of a differential operator to accuracy ε in $O(N \log N \log(1/\varepsilon))$ computer operations and storage. In Sect. 5 we present some applications of MEB to the efficient execution of some typical computational tasks involving the Schrödinger eigenproblem, as well as more general classes of eigenproblems.

In the spirit of electronic structure computations [11,18], we consider (1) with a potential $V(x)$ containing N "features" (e.g., wells), over a spatial periodicity cell $\Omega = [0, L], L = O(N)$, and a fixed energy domain $[\lambda_{\min}, \lambda_{\max}]$ of interest.

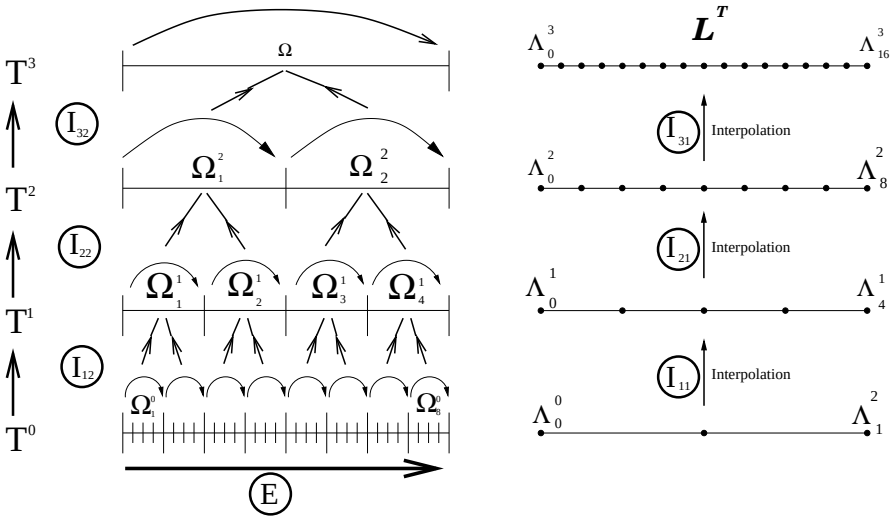

Fig. 1. A four-level ($m = 4$) MEB construction algorithm. The algorithm executes the steps $(E), (I_{11}), (I_{12}), \ldots, (I_{m1}), (I_{m2})$

The MEB consists of $m+1 = O(\log N)$ levels $\{T^l\}_{l=0}^m$; each T^l embodies $n_l \times (k_l+1)$ monodromy functions $\left\{\{\boldsymbol{M}(\Omega_j^l, \Lambda_t^l)\}_{j=1}^{n_l}\right\}_{t=0}^{k_l}$, where $\cup_{j=1}^{n_l}\Omega_j^l = \Omega$, $\Lambda_t^l = \lambda_{\min} + t(\lambda_{\max} - \lambda_{\min})/k_l$, $n_l = 2^{-l}n_0$ and $k_l = 2^l k_0$, so that $n_l \cdot k_l$ is constant throughout stages $l = 0, \ldots, m$.

The MEB construction consists of the following stages (the precise algorithm can be found in [14,15]):

(E) *Evaluation:* for each Λ_t^0, we discretize (2) in each interval Ω_j^0 and use a marching scheme to approximate the monodromy matrix $\boldsymbol{M}(\Omega_j^0, \Lambda_t^0)$. By the complementary smoothness principle, a small k_0 suffices to resolve well the dependence on λ, since Ω_j^0 are of short length (see Fig. 1). Consequently, the computed monodromies can be interpolated to any other $\lambda \in [\lambda_{\min}, \lambda_{\max}]$ with any desirably small interpolation error.

(I_{11}) *Interpolation:* in particular, $\{\boldsymbol{M}(\Omega_j^0; \Lambda_t^0)\}_{j=1,t=0}^{n_0,k_0}$ can be interpolated to a λ-lattice twice as fine, obtaining $\{\boldsymbol{M}(\Omega_j^0; \Lambda_t^1)\}_{j=1,t=0}^{n_0,k_1}$.

(I_{12}) *Merging:* since $\Omega_j^1 := \Omega_{2j-1}^0 \cup \Omega_{2j}^0$, we can calculate

$$\boldsymbol{M}(\Omega_j^1; \Lambda_t^1) := \boldsymbol{M}(\Omega_{2j}^0; \Lambda_t^1) \cdot \boldsymbol{M}(\Omega_{2j-1}^0; \Lambda_t^1) \tag{6}$$

for $j = 1, \ldots, n_1,\ t = 1, \ldots, k_1$. The new monodromies, of spatial intervals twice as large, are smooth on the finer λ lattice.

(I_{21}), ... *Recursion:* since the monodromies of level 1 are smooth on their lattice, they can be interpolated to a finer lattice and then merged to monodromies of intervals twice as large, yielding $\{\boldsymbol{M}(\Omega_j^2; \Lambda_t^2)\}_{j,t}$. The stages of interpolating and merging are repeated until the monodromy of Ω is reached on the appropriate λ resolution.

A precise analysis of errors [14, Sect. 4.2.1] indicates that a minimal amount of work per fixed error ε is attained for $p \le O(\log(N/\varepsilon)), q \le O(\log(N/\varepsilon))$, where p is the discretization order at step (E), and q is the interpolation order of monodromies (steps (I_{l1})). The complexity of the MEB construction is bounded by $O(N(\log N)^2 \log(1/\varepsilon))$. In actual cases (where errors do not always reinforce each other), $p = O(q) = O(\log(1/\varepsilon))$ prove to be satisfactory. Consequently, the MEB construction requires in practice only $O(N \log N \log(1/\varepsilon))$ operations.

5 MEB Applications

The MEB structure is the basis for the efficient execution of general eigenbasis computations. Here we briefly list some of its applications. For a complete description, see [14, Chaps. 4–5].

– *Fast Electronic Density Integration (FEDI).* The Kohn-Sham equations of Density Functional Theory [3,18] involve the computation of the *electronic density* $\varrho(x)$ of the periodic Schrödinger operator, whose integrals

are used to determine the self-consistent potential function $V(x)$ in the nonlinear version of the Schrödinger equation. It is possible to compute ϱ in only $O(N \log N \log(1/\varepsilon))$ operations, using the MEB structure and the fast multilevel summation algorithm [5].

– *Discrete eigenvalue evaluations.* A common computational task in eigenproblems is evaluating the smallest N eigenvalues of a general 1D differential operator with general boundary conditions. The eigenvalues are the roots of an equation involving the entries of the monodromy transformation on the full spatial domain (e.g., (4)). Once the MEB structure has been constructed for the operator, we can evaluate any eigenvalue to an accuracy ε in $O(\log(1/\varepsilon))$ computer operations, regardless of the specific boundary conditions [14, Sect. 4.2.1].
– *Fast expansion in discrete eigenfunctions.* The FEDI algorithm can be applied for computing N coefficients

$$\hat{f}_n := (f, u_n) = \frac{1}{L} \int_0^L f(x) \overline{u_n(x)} dx, \quad n = 1, \ldots, N$$

of the expansion

$$f(x) = \sum_{n=1}^{N} \hat{f}_n u_n = \sum_{n=1}^{N} (f, u_n) u_n$$

to an accuracy ε in $O(N \log N \log(1/\varepsilon))$ operations, where $\{u_n\}_{n=1}^N$ are the eigenfunctions corresponding to the smallest N eigenvalues $\{\lambda_n\}_{n=1}^N$ of a general 1D linear differential operator. Similarly, inverse transforms can be computed to an ε-accuracy in $O(N \log N \log(1/\varepsilon))$ operations [14, Sect. 5.3]. In particular, it is possible to expand fast in eigenfunctions of general self-adjoint Sturm-Liouville eigenproblems

$$(P(x)u'(x))' + Q(x)u(x) = \lambda R(x)u(x) \,, \tag{7}$$

which are of particular interest in mathematical physics. These fast transforms also generalize the FFT algorithm (the case of $Q \equiv 0, P = R \equiv 1$) [14, Sect. 4.2.1].
– *Fast computation of moments.* The FEDI algorithm can be extended to the computation of moments, namely,

$$\mu_n := \frac{1}{L} \int_0^L |u(x; \lambda_n)|^\kappa dx, \quad n = 1, \ldots, N \,,$$

which are important in applications to photonic and phononic crystals [13] (typical values for κ are $2, 4$). The computational complexity of calculating $\{\mu_n\}_{n=1}^N$ to accuracy ε is $O(\kappa^2 N \log N \log(1/\varepsilon))$ [14, Sect. 5.4].

6 Summary and Generalizations

In this paper we presented a class of fast eigenbasis algorithms, based on the multiscale eigenbasis structure for the collective representation of eigenfunctions.

These algorithms are *not limited to localized electronic structures* of quantum chemistry, and can be shown to be *highly parallelizable*. Although we are mainly motivated by ab-initio chemical problems, these algorithms address a much broader variety of 1D expansions in orthogonal systems of general linear differential operators, with general boundary conditions, on general (non-uniform) grids.

Our main future research direction is concerned with the generalization of our 1D algorithms to higher dimensional problems, which are of great importance in condensed matter physics. Although not trivial, indirect higher-dimensional generalizations of our 1D devices do exist.

- In a higher dimension, the concept of a monodromy on a given interval should be replaced by that of a *finite-difference equation* on a comparable meshsize. Analogous to the construction of monodromies of larger intervals from those of smaller intervals (by multiplication), a coarse grid difference equation can be constructed from the next-finer-grid difference equations, using only a certain local set of the latter. The error in the constructed coarse equations decreases *exponentially* with the size of that local set. General algebraic approaches and examples for such constructions are described in [6].
- Finite-difference equations could of course be also used in the *one-dimensional* problem. In the present study the main reason that monodromies were used instead is a certain complication associated with the construction of coarse equations for *highly indefinite* equations. Indeed, for a large meshsize H and for the main range of λ values (those for which $(\lambda - V(x))H^2$ is not small), (1) is highly indefinite on scale H. Specifically, for each such value of λ, solutions of (1) are too oscillatory to be directly represented, even locally, on a grid with such a meshsize. Instead, MEB algorithms should employ a construction similar to the method developed in [8]. The yet unknown solution $u^H(x)$ is expanded as

$$u^H(\boldsymbol{x}) = \sum_{m=1}^{M} a_m^H(\boldsymbol{x}) w_m^H(\boldsymbol{x}) \ . \tag{8}$$

  The $w_m^H(\boldsymbol{x})$ are *known oscillatory* "basis functions", found by relaxing at the fine levels the "root equation"

$$\partial_{\boldsymbol{\xi}} w(\boldsymbol{x}) + i(\lambda - V(\boldsymbol{x}))^{1/2} w(\boldsymbol{x}) = 0 \ , \tag{9}$$

  where $\boldsymbol{\xi}$ is the "propagation direction" associated with the particular basis function w; each basis function of a coarse level is constructed by *locally*

recombining *neighboring* basis functions of the next finer level ("locally" meaning in space $\boldsymbol{x}$, whereas "neighboring" denotes close eigenvalue and propagation direction). The functions $a_m^H(\boldsymbol{x})$ are *smoothly varying, yet unknown* "amplitudes". These *amplitudes are to be calculated on grid* H; for each of them we can construct an equation on grid H, using a local set of the next-finer-grid equations.

– The expansion of the form (8) for each eigenfunction should include only a number (M) of terms which is independent of H, even for $d > 1$. This can be achieved since the known functions $w_m^H(\boldsymbol{x})$ provide a suitable basis of local approximate eigenfunctions on each scale. The local accuracy obtained by relaxation is enough, since the basis functions are subsequently modified by the coarse-level smooth amplitudes. However, the number of different basis functions (or different finite-difference equations) for each value of λ scales linearly with H^{d-1}. At the same time, the number of different λs represented on grid H will be $O(H)$, as with 1D. Thus, the total number of basis functions represented on grid H will be $O(H^d)$.

This outline implies that before tackling higher dimensional extensions of the MEB algorithms, special studies should be first conducted on the following two types of tasks:

1. 1D MEB algorithms based on finite-difference equations instead of monodromies.
2. Extensions of the wave-equation algorithms of [8] to non-constant coefficients, and possibly to more general boundary conditions. The cases of discontinuous coefficients and/or boundary singularities are particularly challenging. However, in applications to electronic-structure problems we do not usually encounter such extreme conditions, since the effective potential is very smooth and boundaries are practically absent.

Having developed MEB structures in higher dimensions, an intriguing question will be whether $O(N \log N)$ computational work is indeed really necessary. It is reasonable to expect that $O(N)$, and sometimes even less, would be enough. First because for many low values of λ, the eigenfunctions are essentially local, lying only in areas where the potential $V(\boldsymbol{x})$ is sufficiently low. On the other hand, for high values of λ, the eigenfunctions approach an asymptotic behavior that can be used to describe them all. At that range of high λs, the main difference between eigenfunctions belonging to different eigenvalues is only in the frequency associated with the base functions, a quantity that can be singled out of the equations by choosing an appropriate form for those functions. Thus, it is expected that the amount of work will not really depend on $\lambda_{\min}$ and $\lambda_{\max}$, but instead will be only proportional to the number of discrete variables needed to resolve the potential $V(\boldsymbol{x})$; that is, *the work is expected to be proportional to the number of atoms.*

For very large structures, even that amount of work may not be needed, since such structures are usually highly *repetitive*. Once coarse-level *equa-*

tions have been constructed, they can be used in other areas where the potential repeats itself (unlike coarse-level *solutions*, which cannot generally be re-used). This aspect is emphasized in other papers on multiscale methods [1,12,21]. In [1], for example, coarse-level Hamiltonians for polymer chains are constructed using local simulations with fine-level Hamiltonians, which are assumed to be known. In a similar manner, the fine-level Hamiltonians themselves (the force field) could presumably be constructured, once and for all, by using local simulations with electronic-structure dynamics.

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References

1. Bai, D. and Brandt, A.: Multiscale computation of polymer models, in: Proceedings of the NATO Advanced Research Workshop on Multiscale Methods in Chemistry and Biology, Eilat, April 5–11 (in press)
2. Bernasconi J., and Schneider, T. (Eds.) Physics in One Dimension, Proceedings of an International Conference at Fribourg, Switzerland, August 25–29, 1980. Springer, Berlin
3. Bernholc, J. and Fattebert, J. L. : Towards grid-based $O(N)$ DFT methods: optimized non-orthogonal orbitals and multigrid acceleration. Physical Review B **62(3)** (2000) 1713–1722
4. Brandt, A.: Multigrid Techniques: 1984 Guide, with Applications to Fluid Dynamics, Available as GMD Studien Nr. 85, from GMD-AIW, postfach 1240, D-5205, St. Augustin 1, West Germany, 1984
5. Brandt, A.: Multilevel computations of integral transforms and particle interactions with oscillatory kernels. Comp. Phys. Comm. **65** (1991) 24–38
6. Brandt, A.: General highly accurate algebraic coarsening. Elec. Trans. Num. Anal. **10** (2000) 1–10
7. Brandt, A.: Multiscale Scientific Computation 2000. These Proceedings
8. Brandt, A. and Livshits, I.: Wave-ray multigrid method for standing wave equations. Elec. Trans. Num. Anal. **6** (1997) 162–181
9. Brandt, A., McCormick, S. and Ruge, J.: Multigrid methods for differential eigenproblems, SIAM J. Sci. Stat. Comput. **4** (1983) 244–260
10. Costiner, S. and Ta'asan, S.: Adaptive multigrid techniques for large-scale eigenvalue problems: Solutions of the Schrödinger problem in two and three dimensions. Physical Review E **51(4)** (1995) 3704–3717
11. Gödecker, S.: Linear scaling electronic structure methods. Reviews of Modern Physics **71(4)** (1999) 1085–1123
12. Ilyin, V. and Brandt, A.: Multilevel approach in statistical physics of liquids, in: Proceedings of the NATO Advanced Research Workshop on Multiscale Methods in Chemistry and Biology, Eilat, April 5–11 (in press)

13. Joannopolous, J. D., Meade, R. D. and Winn, J. N.: Photonic Crystals, Princeton University Press, Princeton, New Jersey, 1995
14. Livne, O. E.: Multiscale Eigenbasis Algorithms. Ph. D. Thesis, Weizmann Institute of Science, Rehovot, 2000
15. Livne, O. E. and Brandt, A.: $O(N \log N)$ multilevel calculation of N eigenfunctions, in: Proceedings of the NATO Advanced Research Workshop on Multiscale Methods in Chemistry and Biology, Eilat, April 5–11 (in press)
16. Manakov, S. V., Novikov, S .P., Pitaevskij, L. P. and Zakharov, V.E. Theory of Solitons: The Inverse Problem Method, Nauka, Moscow. English transl.: Consultants Bureau, New York, 1984
17. Parlett, B. N.: The Symmetric Eigenvalue Problem, Prentice-Hall, Englewood Cliffs, New Jersey, 1980
18. Parr, R.G. and Yang, W.: Density-Functional Theory of Atoms and Molecules, Oxford University Press, New York, 1989
19. Shubin, M.A. (Ed.): Partial Differential Equations VII: Spectral Theory of Differential Operators, Springer, Berlin, 1994
20. Slater, J.: Quantum Theory of Molecules and Solids, McGraw-Hill, New York, 1963
21. Ron, D. and Brandt, A.: Renormalization multigrid (RMG): Coarse-to-fine Monte Carlo acceleration and optimal derivation of macroscopic actions, in: Proceedings of the NATO Advanced Research Workshop on Multiscale Methods in Chemistry and Biology, Eilat, April 5–11 (in press)
22. Ziman, J.M.: Principles of the Theory of Solids, Cambridge University Press, Cambridge, 1972