FEAST for Complex Band Structure Problems

S.E. Laux
IBM Research Division
T.J. Watson Research Center
P.O. Box 218
Yorktown Heights, NY 10598-0218
E-mail: laux@us.ibm.com

***Abstract*—The FEAST eigenvalue algorithm of Polizzi [1] is extended to solve the complex band structure problem.**

I. Motivation

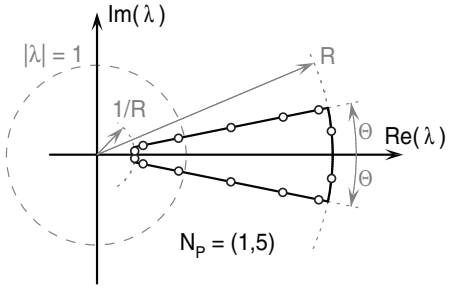
The complex band structure problem (or equivalently, the scatttering-states problem [2]) poses a unique computation challenge: in addition to matrix order N potentially being very large, the generalized eigenvalue problem (GEP) $\boldsymbol{A}x = \lambda \boldsymbol{B}x$ involves matrices $\boldsymbol{A}$, $\boldsymbol{B}$ which are complex-valued, non-Hermitian, and possibly singular (as is the case here). The FEAST algorithm [1] is straightforwardly extended to a dual subspace variant [3], [4] (required for non-Hermitian matrices) and intrepidly invoked. The results are very positive: in cases where matrices are sparse, few eigenvalues are sought, and especially where a sequence of related systems are considered such that initial guesses become available, the algorithm performs remarkably.

II. Model Problem and Discussion

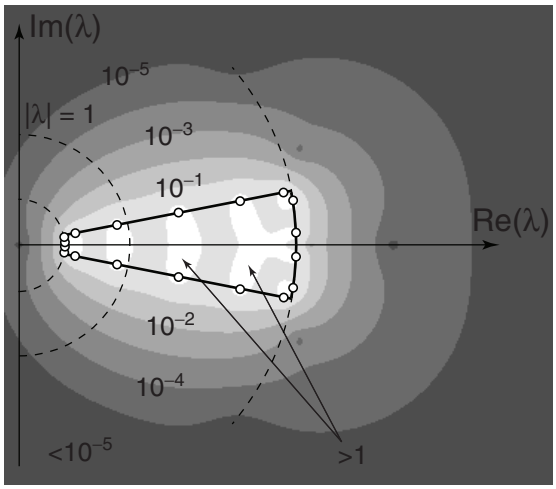
The model problem is to compute the complex band structure [5] (with zone unfolding [6], [7]) of Si layers of varying thicknesses. Thicknesses in the [001] z-direction range from 37 atomic layers ($N = 3312$) to 2557 atomic layers ($N = 204912$) with transport in the [100] x-direction; $k_y = 0$. An $sp^3d^5s^*$ Hamiltonian including spin-orbit interaction is used [8]; dangling bonds are H terminated [9].

Only the first few (≥ 8) complex-valued wavevectors *with minimum* $Im(|k_x|) > 0$ are sought at each given energy; within the bandgap this obtains the loci of least action for band-to-band tunneling [10]. Since $\lambda = e^{\imath k_x L}$ (L the unit cell size) [5], a suitable FEAST contour is shown Fig. 1(a). $R > 1$ is adjusted to capture these solutions and must be quite precise: R too small and no eigenvalues are obtained; too large and far too many eigenvalues are erroneously sought.

FEAST converges in *one iteration* if the contour integration of the Green's function ((3) of [1]) is exact. Using Gauss-Legendre quadrature (GLQ) usually precludes this. GLQ defines a (here novel) 'selection function' $S(\lambda)$ which represents a filter to accept or reject eigenvalues. Ideally, S is unity within the contour and zero elsewhere; in practice this is only achieved when many quadrature points are used. Fig. 1(b) shows S for realistic N_P.



(a)



(b)

Fig. 1. (a) Prototype FEAST contour. N_P=$(1, 5)$ indicates the number of Gauss-Legendre quadrature points around the contour: here one on each of four sections of constant radius, and five on each of two sections of constant angle (total 14). (b) $S(\lambda)$ plotted for R=2.5, Θ=0.2 and N_P=$(2, 5)$. S is approximately unity within the contour, does not fall off with infinite abruptness outside the contour and is singular at GLQ point locations.

III. Results

Physics and numerics results are shown in Fig. 2 for the $N = 204912$ problem. The path of least action is depicted in the left panel using 151 energy points. In the right panel, relatively few FEAST iterations are required in the energy gap of Si because a reasonble initial guess is available (not so in the conduction and valence bands). The number of quadrature points N_P increases in the gap to track the contour's R increase required by the increase in the minimum value of $Im(|k_x|)$. The number of eigenvalues resolved stays small

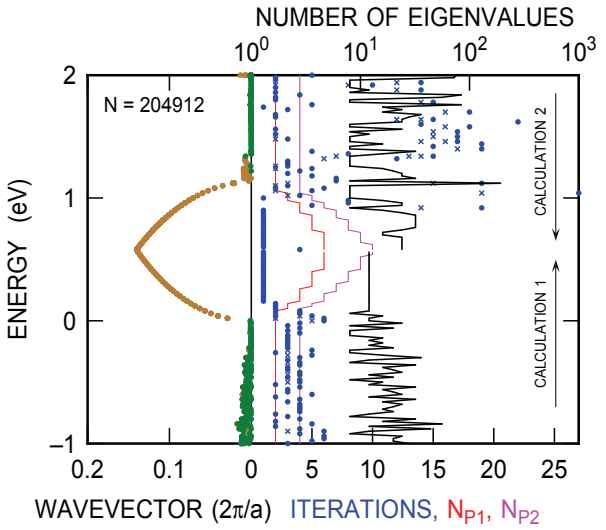


Fig. 2. (left) Energy *vs.* $Im(k_x)$; both pure imaginary (brown) and complex-valued (green) wavevectors are seen. (right) Iterations required ($\times$ R adjustment taken; $\bullet$ final; blue), N_P (red, magenta), and number of eigenvalues obtained for a given energy (black).

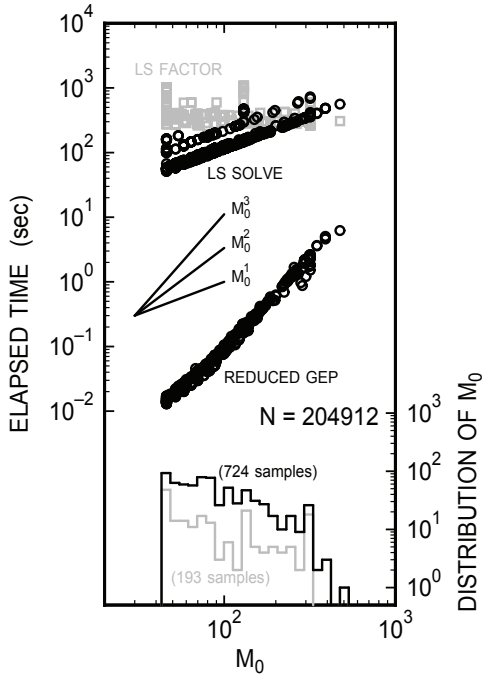


Fig. 3. Verification that reduced GEP solution ($\propto M_0^3$) remains insignificant compared to linear system (LS) factorizations ($\propto M_0^0$) and backsolutions ($\propto M_0^1$). This is accomplished by keeping M_0 small; distributions for M_0 used for factorization (gray) and otherwise (black) are shown.

(< 220) as it must to keep M_0 small.

Fig. 3 verifies that linear system (LS) factorization and solve times dominate reduced GEP times. As such, as N increases, FEAST performance is determined by LS growth rates which is the entire rational behind FEAST – replacing a large GEP with a small GEP and many LSs [1].

Rather than just quoting parallel performance, Fig. 4 gives timing and storage information for the computationally intense

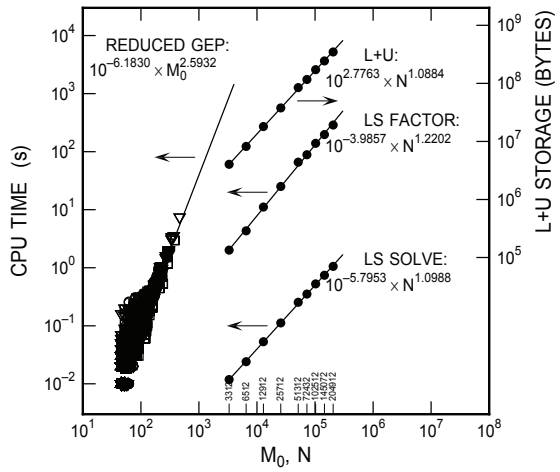


Fig. 4. Timing and storage requirements of computationally intensive FEAST ingredients. Reduced GEP solve time is nearly cubic in M_0. Linear system factor, solve and storage are nearly linear in N, consistent with the sparsity of the model problem.

ingredients of FEAST. In computing all of Fig. 2, at each FEAST iteration *on average* 41.3 independent matrices are simultaneously available for factorization (range 32–88) and 105.5 independent right-hand side vectors are available for backsolution (range 46-474). The opportunity for significant parallization is obvious; here a 27.1 speedup on 32 processors is obtained. Ideal speedup is not obtained because both LS factors and solves are sequential processes [11] (and modified for complex arithmetic), with the number required generally not a multiple of 32.

References

[1] E. Polizzi, "Density–matrix–based algorithm for solving eigenvalue problems," *Phys. Rev. B*, vol. 79, no. 11, p. 115112, 2009.

[2] M. Luisier, A. Schenk, W. Fichtner, and G. Klimeck, "Atomistic simulation of nanowires in the sp^3d^5s* tight-binding formalism: From boundary conditions to strain calculations," *Phys. Rev. B*, vol. 74, no. 20, p. 205323, 2006.

[3] E. Polizzi, Private communication, 2009.

[4] P. M. Morse and H. Feshbach, *Methods of Theoretical Physics Part I: Chapters 1 to 8*. New York, NY: McGraw-Hill, 1953.

[5] T. B. Boykin, "Generalized eigenproblem method for surface and interface states: The complex bands of GaAs and AlAs," *Phys. Rev. B*, vol. 54, no. 11, p. 8107, 1996.

[6] T. B. Boykin and G. Klimeck, "Practical application of zone-folding concepts in tight binding calculations," *Phys. Rev. B*, vol. 71, no. 11, p. 115215, 2005.

[7] A. Ajoy, K. V. R. M. Murali, and S. Karmalkar, "Brillouin zone unfolding of complex bands in a nearest neighbour tight binding scheme," *J. Phys.: Condens. Matter*, vol. 24, no. 5, p. 055504, 2012.

[8] T. B. Boykin, G. Klimeck, and F. Oyafuso, "Valence band effective-mass expressions in the sp^3d^5s* empirical tight-binding model applied to a Si and Ge parametrization," *Phys. Rev. B*, vol. 69, no. 11, p. 115201, 2004.

[9] Y. Zheng, C. Rivas, R. Lake, K. Alam, T. B. Boykin, and G. Klimeck, "Electronic properties of silicon nanowires," *IEEE Trans. Electron Dev.*, vol. 52, no. 6, pp. 1097–1103, 2005.

[10] S. E. Laux, "Computation of complex band structures in bulk and confined structures," in *Proc. 13th Int. Workshop on Computational Electronics*. Piscataway, NJ: IEEE, 2009, pp. 5–8.

[11] Z. Zlatev, J. Wasniewski, and K. Schaumburg, *Y12M, Solution of Large and Sparse Linear Algebraic Equations*, ser. Lecture Notes in Computer Science. New York/Heidelberg: Springer-Verlag, 1981, no. 121, code available at www.netlib.org/y12m.