

# FEAST for Complex Band Structure Problems

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## MOTIVATION

The complex band structure problem (or equivalently, the scattering-states problem [1]) poses a unique computation challenge: in addition to matrix order  $N$  potentially being very large, the generalized eigenvalue problem (GEP)  $Ax = \lambda Bx$  involves matrices  $A$ ,  $B$  which are complex-valued, non-Hermitian, and possibly singular (as is the case here). The FEAST algorithm [2] 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.

## 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 ( $\geq 8$ ) complex-valued wave-vectors *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  $\lambda = e^{ik_x L}$  ( $L$  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 [2]) 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  $N_P$ .

## 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 reasonable 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 ( $< 220$ ) 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 rationale behind FEAST – replacing a large GEP with a small GEP and many LSs [2].

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

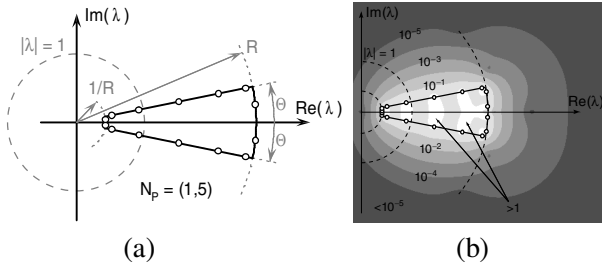


Fig. 1. (a) Prototype FEAST contour.  $N_P=(1,5)$  indicates the number of Gauss-Legendre quadrature points around the contour: here one on each of four sections of constant radius, and five on each of two sections of constant angle (total 14). (b)  $S(\lambda)$  plotted for  $R=2.5$ ,  $\Theta=0.2$  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.

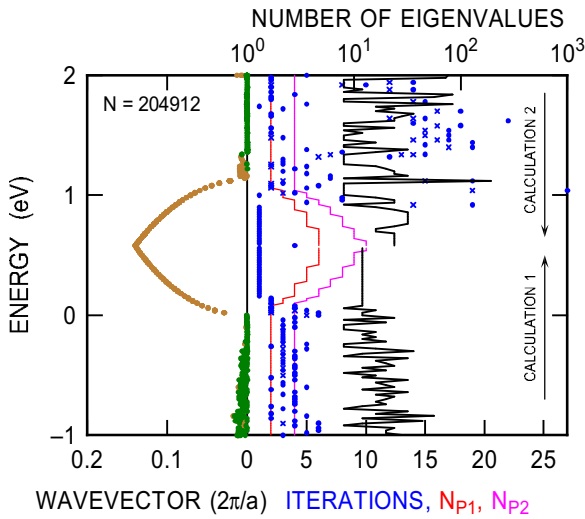


Fig. 2. (left) Energy vs.  $Im(k_x)$ ; both pure imaginary (brown) and complex-valued (green) wavevectors are seen. (right) Iterations required ( $\times R$  adjustment taken;  $\bullet$  final; blue),  $N_P$  (red, magenta), and number of eigenvalues obtained for a given energy (black).

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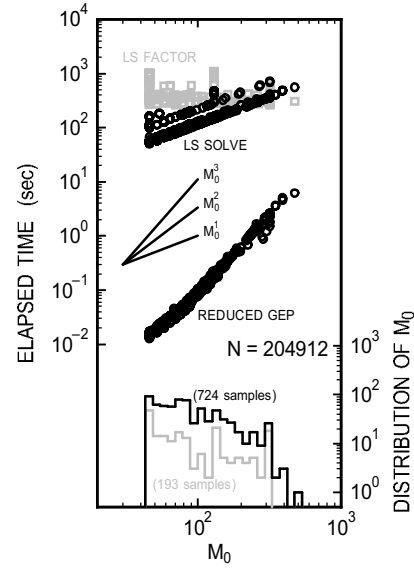


Fig. 3. Verification that reduced GEP solution ( $\propto M_0^3$ ) remains insignificant compared to linear system (LS) factorizations ( $\propto M_0^0$ ) and backsolutions ( $\propto M_0^1$ ). This is accomplished by keeping  $M_0$  small; distributions for  $M_0$  used for factorization (gray) and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

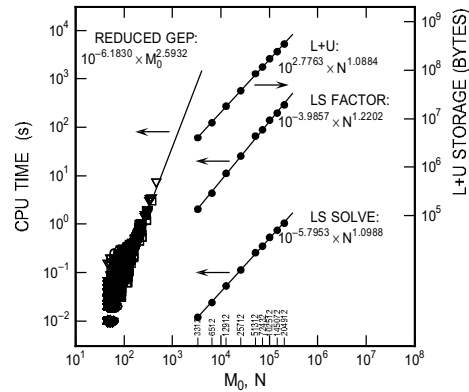


Fig. 4. Timing and storage requirements of computationally intensive FEAST ingredients. Reduced GEP solve time is nearly cubic in  $M_0$ . Linear system factor, solve and storage are nearly linear in  $N$ , consistent with the sparsity of the model problem.