

# **Bounding the Spectrum of Large Hermitian Matrices**

**Ren-Cang Li  
Yunkai Zhou**

**Technical Report 2009-07**

# Bounding the Spectrum of Large Hermitian Matrices

Ren-Cang Li\* and Yunkai Zhou†

May 30, 2009

*Dedicated to Prof. G. W. Stewart on the occasion of his 70th birthday*

## Abstract

Estimating upper bounds of the spectrum of large Hermitian matrices has long been a problem with both theoretical and practical significance. Algorithms that can compute tight upper bounds with minimum computational cost will have applications in a variety of areas. We present a practical algorithm that exploits  $k$ -step Lanczos iteration with a safeguard step. The  $k$  is generally very small, say 5 to 8, regardless of the large dimension of the matrices. This makes the Lanczos iteration economical. The safeguard step can be realized with marginal cost by utilizing the theoretical bounds developed in this paper. The bounds establish the theoretical validity of a previous bound estimator that has been successfully used in various applications. Moreover, we improve the bound estimator which can now provide tighter upper bounds with negligible additional cost.

**Key words:** Hermitian matrix, Largest eigenvalue, upper bound, Lanczos

## 1 Introduction

Various researchers have studied cost-effective ways to approximate the largest eigenvalue of Hermitian matrices. O’Leary, Stewart, and Vandergraft [11] used Rayleigh-quotient iteration; Parlett, Simon, and Stringer [12], and Kuczyński and Woźniakowski [10] employed Lanczos iteration with random initial vectors. The focus in [11, 12, 10] is to make rather accurate estimate of the largest eigenvalue of Hermitian positive definite matrices. Because the estimation is expected to have high accuracy, the iteration steps often cannot be very small.

In contrast, in several applications we cannot afford to estimate the largest eigenvalue to high accuracy because it can be too costly, especially when the estimation procedure has to be done repeatedly in a single simulation. Instead, we focus on obtaining practical upper bounds of the spectrum with low cost. Our upper bound estimator is also based on the Lanczos iteration [13, 16]. One major application of our estimator is for the Chebyshev-filtered subspace iteration method [18, 19] in real-space Density Functional Theory (DFT)

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\*Department of Mathematics, University of Texas at Arlington, Arlington, TX 76019 ([rcli@uta.edu](mailto:rcli@uta.edu).) Supported in part by the National Science Foundation under Grant No. DMS-0702335 and DMS-0810506.

†Department of Mathematics, Southern Methodist University, Dallas, TX 75275 ([yzhou@smu.edu](mailto:yzhou@smu.edu).) Supported in part by the National Science Foundation under Grant No. CMMI-0727194 and OCI-0749074.

calculations, where an estimator for the largest eigenvalues of some Hermitian matrices has to be repeatedly called for. The Hermitian matrices arise from real-space DFT calculations [2] are indefinite, sparse, and usually of very large scale.

The upper bound plays a crucial role for the efficiency of the Chebyshev filters. It is understood that the tighter the upper bound the better. But there is a tradeoff between tightness of a bound and the computational cost for it. The large dimension implies that it is not cost-effective to let the Lanczos iteration run until a Ritz value converges to the largest eigenvalue. Instead we wish to obtain an upper bound within just a few Lanczos steps, say less than 8 steps, regardless of the dimension of the matrices. To achieve this goal we need to look deeper into the bounds from Lanczos iteration and provide necessary safeguard steps.

An inexpensive upper bound estimator was proposed in [18]. The estimator plays a critical role in the nonlinear Chebyshev filtered subspace iteration method that is now the default solver in the real-space DFT package called PARSEC [2, 3]. It has been successfully used for a wide range of DFT calculations, including highly challenging problems with dimension over several millions, where several thousand eigenpairs need to be computed [3, 17, 19]. The application of the estimator is not limited to DFT calculations, e.g., it plays a part in the Chebyshev-Davidson algorithm [20] for solving Hermitian eigenvalue problems of large dimensions.

However, the upper bound estimator in [18] lacks a rigorous proof. In this paper we will analyze the bound in more details, provide certain conditions under which we can rigorously prove that the estimator provides an upper bound. We also develop tighter upper bounds based on our analysis. Moreover, we will construct practical heuristics to guarantee that the estimator will provide an upper bound even if the conditions do not hold. This is important to ensure robustness of the upper bound estimator.

The rest of this article is organized as follows. Section 2 provides a theoretical analysis for practical bounds. Numerical examples, including those from DFT calculations and two artificial ones purposely constructed to test our bounds, are presented in Section 3 to illustrate the effectiveness of the proposed bounds in the previous section. We conclude this article by a few remarks along with possible applications other than DFT calculations in Section 4

## 2 Theoretical Study of Upper Bounds

Denote the size  $n \times n$  Hermitian matrix as  $A$  and  $\lambda_{\max}(A)$  its largest eigenvalue. As explained in [18], the Chebyshev-filtered subspace iteration method requires an upper bound  $\beta$  that satisfies  $\beta \geq \lambda_{\max}(A)$ . Theoretically, any consistent norm  $\|A\|$ , in particular the  $\ell_1$ - or  $\ell_\infty$ -operator norm provides an upper bound on  $\lambda_{\max}(A)$ . Also, Gerschgorin's disk leads to another means. But as pointed out in [18, Section 4.3], upper bounds obtained as such are often too crude to be considered effective for the subspace iteration. Another obstacle associated with these methods occurs when  $A$  is not stored as a matrix but instead accessed via a matrix-vector product subroutine. This is usually the case in DFT calculations, either in real-space or in plane-wave setting.

The upper bound estimator proposed in [18] performs the following: Run  $k$ -step Lanczos [13, 16] on  $A$  with a random starting vector to get

$$AQ_k = Q_k T_k + f_k e_k^T, \quad (2.1)$$

where  $Q_k$  is  $n \times k$  and has orthonormal columns,  $T_k$  is  $k \times k$  and tri-diagonal,  $Q_k^* f_k = 0$ , the superscript  $*$  denotes conjugate transpose (it becomes just transpose in the real case), and  $e_k$  is the  $k$ th column of the  $k \times k$  identity matrix. Then take  $\lambda_{\max}(T_k) + \|f_k\|_2$  as an upper bound on  $\lambda_{\max}(A)$ . While no analysis was presented in [18] to theoretically guarantee that  $\lambda_{\max}(T_k) + \|f_k\|_2$  was indeed an upper bound, we observed that a very small  $k$ , say  $4 \leq k \leq 10$ , was often enough to provide an upper bound.

It is not hard to see that the method can fail if the starting vector is unfortunately taken from an invariant subspace that is orthogonal to  $A$ 's eigenspace corresponding to  $\lambda_{\max}(A)$ . But the initial vector is randomly generated, nowadays any random number generator (see [9]) used would make this scenario a probability zero incidence. Hence in practice we can safely assume that the random initial vector is not orthogonal to the eigenspace corresponding to  $\lambda_{\max}(A)$ .

Now we shall present conditions that guarantee  $\lambda_{\max}(T_k) + \|f_k\|_2$  to be an upper bound on  $\lambda_{\max}(A)$ . Then we proceed to develop some refined bounds.

Denote the eigenvalues of  $A$  and  $T_k$  by

$$\lambda_1 \leq \lambda_2 \leq \dots \leq \lambda_n \quad \text{and} \quad \mu_1 \leq \mu_2 \leq \dots \leq \mu_k,$$

respectively.

In exact arithmetic,  $Q_k$  in (2.1) has orthonormal columns, i.e.,  $Q_k^* Q_k = I_k$ . Numerically,  $Q_k$ 's columns are nearly orthonormal for  $k$  not too big. It is well-known that the orthogonality among  $Q_k$ 's columns begins to deteriorate as  $T_k$ 's eigenvalues start to converge to  $A$ 's [13, Section 13.3]. But as pointed out in [18], for the purpose of bounding  $\lambda_{\max}(A)$ , only very few steps, i.e., small  $k$ , suffices. Because of that, the Lanczos process would usually stop far before  $\lambda_{\max}(T_k)$  approximates one of  $A$ 's eigenvalues accurately. Moreover, the randomly selected initial vector most likely ensure that  $\lambda_{\max}(T_k)$  would be closer to  $\lambda_{\max}(A)$  than to other eigenvalues of  $A$ . Therefore it is reasonable to assume that after a few Lanczos steps,

$$|\lambda_n - \lambda_{\max}(T_k)| = \min_i |\lambda_i - \lambda_{\max}(T_k)|. \quad (2.2)$$

It is also reasonable to assume that for  $k$  not too big,  $Q_k$ 's columns are nearly orthonormal.

**Lemma 1** (Kahan [7], Cao, Xie, and Li [1]). *There exist  $k$  eigenvalues of  $A$ :  $\lambda_{i_1} \leq \lambda_{i_2} \leq \dots \leq \lambda_{i_k}$  such that*

$$|\lambda_{i_j} - \mu_j| \leq \frac{\|f_k\|_2}{\sigma_{\min}(Q_k)}$$

for  $1 \leq j \leq k$ , where  $\sigma_{\min}(Q_k)$  is the smallest singular value of  $Q_k$ .

This lemma holds regardless of the assumption (2.2) and orthogonality among  $Q_k$ 's columns. But if  $Q_k$ 's columns are nearly orthonormal, then  $\sigma_{\min}(Q_k) \approx 1$ .

**Theorem 1.** *If (2.2) holds, then*

$$\lambda_{\max}(A) \leq \lambda_{\max}(T_k) + \frac{\|f_k\|_2}{\sigma_{\min}(Q_k)}. \quad (2.3)$$

*Proof.* With (2.2), one can take  $i_k = n$  in Lemma 1. Then

$$\lambda_{\max}(A) = \lambda_n \leq \mu_k + \frac{\|f_k\|_2}{\sigma_{\min}(Q_k)} = \lambda_{\max}(T_k) + \frac{\|f_k\|_2}{\sigma_{\min}(Q_k)},$$

as expected. □

A sharper bound than (2.3) is given in the next theorem.

**Theorem 2.** *Suppose (2.2) holds. Let  $T_k z = \mu_k z$  and  $\|z\|_2 = 1$ . Then*

$$\lambda_{\max}(A) \leq \lambda_{\max}(T_k) + \frac{|e_k^T z| \|f_k\|_2}{\|Q_k z\|_2}. \quad (2.4)$$

*Proof.* Multiply  $z$  from the right to the equation (2.1) to get

$$A Q_k z - \mu_k Q_k z = f_k e_k^T z.$$

With (2.2), we have [13, p.73]

$$\lambda_{\max}(A) = \lambda_n \leq \mu_k + \frac{\|f_k e_k^T z\|_2}{\|Q_k z\|_2} = \lambda_{\max}(T_k) + \frac{|e_k^T z| \|f_k\|_2}{\|Q_k z\|_2},$$

as expected. □

We make the following remarks:

1. Since  $|e_k^T z| \leq 1$  and  $\|Q_k z\|_2 \geq \sigma_{\min}(Q_k)$ , (2.3) is a consequence of (2.4).
2. It is argued that for small  $k$   $Q_k$ 's columns are usually nearly orthonormal, which ensures both  $\sigma_{\min}(Q_k)$  and  $\|Q_k z\|_2$  are very much 1. Therefore the right-hand sides of (2.3) and of (2.4) are essentially

$$\lambda_{\max}(T_k) + \|f_k\|_2, \quad (2.5)$$

$$\lambda_{\max}(T_k) + |e_k^T z| \|f_k\|_2, \quad (2.6)$$

respectively, for the practical purpose. This, in a way, justifies the validity of using  $\lambda_{\max}(T_k) + \|f_k\|_2$  as an upper bound on  $\lambda_{\max}(A)$  in [18].

3. There is no assumption made in Theorems 1 and 2 for  $\lambda_{\max}(A)$  to be a simple eigenvalue. It can be a multiple eigenvalue.
4. Although our goal is to have upper bound estimates for  $\lambda_{\max}(A)$ , one readily has  $\lambda_{\max}(A) \geq \lambda_{\max}(T_k)$  [13, 15], giving a lower bound for  $\lambda_{\max}(A)$ .

5. Similar statements hold for  $\lambda_{\min}(A) = \lambda_1$ . By applying the results above to  $-A$ , we can have economical ways to bound  $\lambda_{\min}(A)$ , both from below and from above. In fact, with (2.1) if

$$|\lambda_1 - \lambda_{\min}(T_k)| = \min_i |\lambda_i - \lambda_{\min}(T_k)|,$$

then we have, similarly to Theorems 1 and 2,

$$\begin{aligned} \lambda_{\min}(T_k) - \frac{\|f_k\|_2}{\sigma_{\min}(Q_k)} &\leq \lambda_{\min}(A) \leq \lambda_{\min}(T_k), \\ \lambda_{\min}(T_k) - \frac{|e_k^T z| \|f_k\|_2}{\|Q_k z\|_2} &\leq \lambda_{\min}(A) \leq \lambda_{\min}(T_k), \end{aligned}$$

where  $z$  is the unit eigenvector of  $T_k$  associated with  $\lambda_{\min}(T_k)$ .

It is impractical to verify Assumption (2.2) in actual computations because  $A$ 's eigenvalues  $\lambda_i$  are unknown. But the existing convergence theory (in exact arithmetic) [8, 13, 14] does suggest that if the initial random vector has nontrivial component in the direction of  $A$ 's eigenvector associated with  $\lambda_{\max}(A)$ , then  $\lambda_{\max}(T_k)$  usually converges to  $\lambda_{\max}(A)$  faster than any other  $\mu_i$  to some eigenvalues of  $A$ . Years of numerical practices support the theory, too, in the floating point environment.

Recall that the goal is to obtain a true upper bound. The bound (2.5)  $\lambda_{\max}(T_k) + \|f_k\|_2$  has reliably produced an upper bound on  $\lambda_{\max}(A)$  in all our tests from DFT. The result appears to be not reliant on hypothesis (2.2). In fact we tried matrices from other fields, we also constructed examples difficult for the Lanczos to achieve convergence for the largest eigenvalue, including matrices whose eigenvalues are highly clustered near the largest eigenvalue while smallest eigenvalues dominate in magnitude, but bound (2.5) always provides an upper bound in just a few Lanczos steps.

However, in cases when hypothesis (2.2) fails, occasionally the bound (2.6)  $\lambda_{\max}(T_k) + |e_k^T z| \|f_k\|_2$  derived from Theorem 2 may underestimate  $\lambda_{\max}(A)$ . When it does not underestimate, it gives the sharpest upper bound among all. For the task of robustly providing an upper bound, we propose the following modification to (2.6), which utilizes not just the eigenvector associated with  $\mu_k$ , but instead all the eigenvectors of  $T_k$ . We arrive at the following bound

$$\lambda_{\max}(A) \leq \lambda_{\max}(T_k) + \max_z |e_k^T z| \|f_k\|_2, \quad (2.7)$$

where  $z$  is any unit eigenvector of  $T_k$ . Bound (2.7) works surprisingly well in our tests. One explanation is that the right-hand side of (2.7) is always no smaller than that of (2.6), which means (2.2) in Theorem 2 may be relaxed. Another explanation is that, the scaling factor for  $\|f_k\|_2$  in Theorem 2 is  $\frac{|e_k^T z|}{\|Q_k z\|_2}$ , hence using a scaling factor no less than  $|e_k^T z|$  may provide enhanced safeguard for the rare cases in floating point arithmetic that  $\frac{1}{\|Q_k z\|_2}$  may be close to 1 but smaller than 1. But we feel that a more satisfactory understanding on the choice of  $\max_z |e_k^T z|$  may require further study.

Intuitively, among all the eigenvectors of  $T_k$ , those associated with Ritz values close to  $\lambda_{\max}(T_k)$  (i.e.,  $\mu_{k-2}, \mu_{k-1}, \mu_k$ ) can be more important than those associated with smaller

Ritz values. Therefore we can sharpen (2.7) as

$$\lambda_{\max}(A) \leq \lambda_{\max}(T_k) + \max_{z \in \{z_{k-2}, z_{k-1}, z_k\}} |e_k^T z| \|f_k\|_2, \quad (2.8)$$

where  $z_{k-2}, z_{k-1}, z_k$  are the unit Ritz vectors associated with  $\mu_{k-2}, \mu_{k-1}, \mu_k$ , respectively.

We avoid computing any term that contains the Lanczos vectors  $Q_k$  in all of the bounds (2.5), (2.6), (2.7), and (2.8). This is mainly for saving computational cost. Since  $Q_k$  is of size  $n$  by  $k$  where  $n$  is usually huge, estimating either  $\sigma_{\min}(Q_k)$  or  $\|Q_k z\|_2$  involves non-negligible cost. Moreover,  $Q_k$  does not need to be stored in the Lanczos bound estimator. As discussed above, when  $k$  is small and convergence just starts to happen to a couple of digits at most, we can practically use  $\sigma_{\min}(Q_k) \approx \|Q_k z\|_2 \approx 1$ .

Clearly, if hypothesis (2.2) holds, the bound (2.6) from Theorem 2 is the sharpest, followed by (2.8), then (2.7), and then (2.5). The latter three provide increasingly stronger safeguard to (2.6) in case (2.2) does not hold.

We note that computing eigenvectors of a  $k \times k$  Hermitian tridiagonal matrix  $T_k$  for small  $k$  constitutes only negligible cost, therefore the cost for bounds (2.6), (2.8), and (2.7) are essentially the same as that of (2.5).

### 3 Numerical Study of the Bounds

In this section we provide numerical study of the bounds (2.5), (2.6), (2.7), and (2.8). We'll see that the bound (2.6) works nicely most of the time, especially for problems from real applications. This is mainly due to the efficiency of the Lanczos method that can quickly approximate the exterior eigenvalues, which makes (2.2) valid most of the time, even for a small  $k$ .

The presented results, Figures 3.1 – 3.5, are selected from a large number of tests using matrices<sup>1</sup> from small scale real-space DFT calculations. The dimension of each matrix is noted on the title of each figure. The bounds as functions of the Lanczos step  $k$  shown in the figures are representative behaviors of each bound.

In the legend of each figure, `bnd1`, `bnd2`, `bnd3`, and `bnd4` refer to (2.5), (2.6), (2.7), and (2.8), respectively. The `maxeig` refers to  $\lambda_{\max}(A)$ . The bound (2.6) is often so sharp that we opt not to use a special symbol for `bnd2` so that it does not severely block the line for `maxeig`.

Five dotted vertical lines are drawn for  $k = 4, 5, 6, 7, 8$ , as references to show that the safeguarded bounds quickly become upper bounds of  $\lambda_{\max}(A)$  even after only 4 or 5 Lanczos iterations.

The plots are for  $k$  from 1 to 30. This is for illustration purpose. In real computations, one seldom needs to go over 15 Lanczos steps. With safeguards, normally 7 to 9 steps are good enough for an effective upper bound. Moreover, from the plots we see that performing more Lanczos steps does not necessarily improve the bound much. The more cost-effective approach is to perform less than 10 Lanczos steps and apply appropriate

<sup>1</sup>The matrices are available at the University of Florida Sparse Matrix Collection [4] under the group name "PARSEC".

safeguards. Another point worth mentioning is that, for  $k < 4$ ,  $\lambda_{\max}(T_k)$  has not become a reasonable approximation to  $\lambda_{\max}(A)$ , hence (2.2) can be completely wrong. In this case the safeguards are not strong enough to provide an upper bound. It is necessary to perform a few more Lanczos steps so that (2.2) becomes reasonable, which means the bound (2.6) becomes right or almost right, then the safeguards in (2.8) or (2.7) will provide a safe upper bound that is sharper than (2.5).

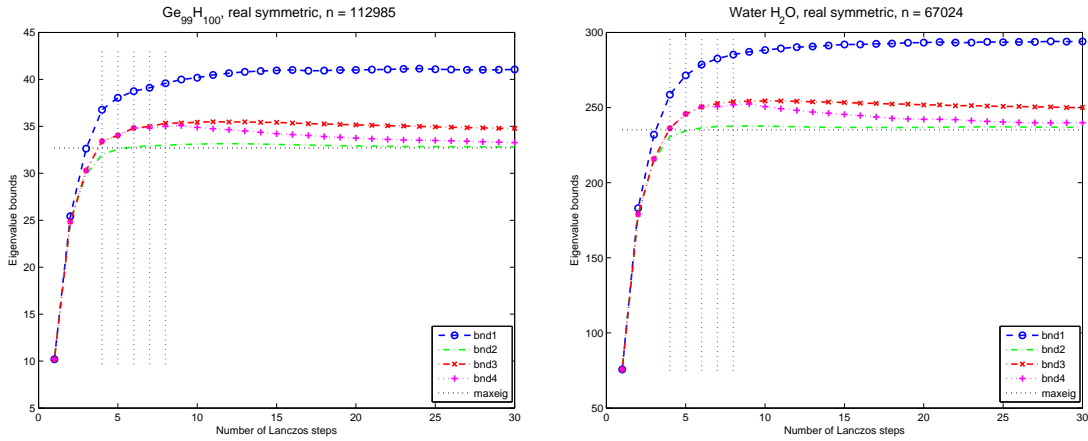


Figure 3.1: Behavior of bounds on a hydrogen passivated germanium clusters  $Ge_{99}H_{100}$  and a water molecular.

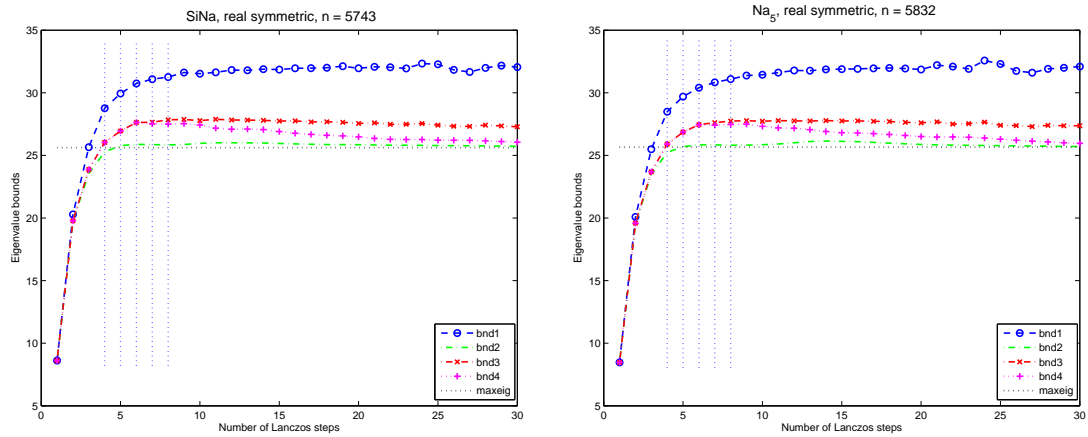


Figure 3.2: Behavior of bounds on  $SiNa$  and  $Na_5$ .

We use a nontrivial example to show that our bounds can handle difficult problems. Figure 3.6 shows the behavior of bounds for two  $10^7 \times 10^7$  diagonal matrices. (Unitary similarity transformation of a diagonal matrix into a nondiagonal matrix does not affect the behavior of Lanczos, so using diagonal matrices does not lose generality.)

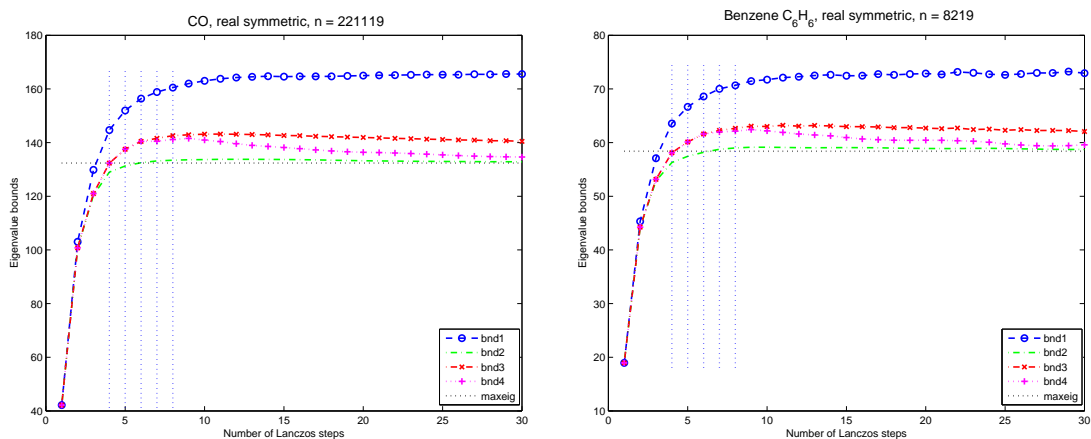


Figure 3.3: Behavior of bounds on a carbon monoxide  $CO$  molecular and the Benzene  $C_6H_6$  molecular.

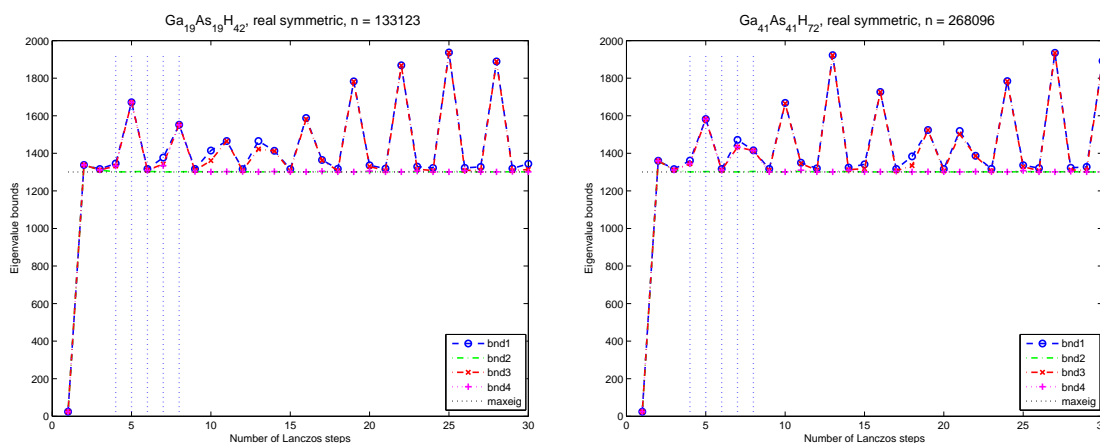


Figure 3.4: Behavior of bounds on two hydrogen passivated gallium arsenide clusters  $Ga_{19}As_{19}H_{42}$  and  $Ga_{41}As_{41}H_{72}$ . These two examples have a distinct feature: three largest eigenvalues dominate in magnitude and are clustered. As seen from this plot, the safeguards used for **bnd1** and **bnd3** are conservative and may give too large upper bound at some steps. Clearly for these two bounds more Lanczos steps do not translate into sharper bounds. While **bnd2** and **bnd4** very much collapse onto **maxeig** after  $k = 4$ , which also shows that more Lanczos steps are not necessary if an appropriate safeguard is applied.

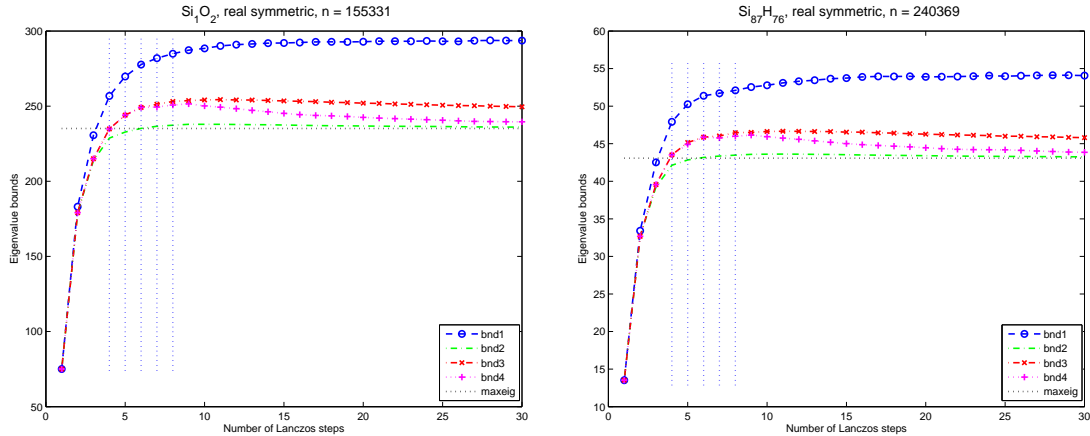


Figure 3.5: Behavior of bounds on silicon dioxide  $SiO_2$  and hydrogen passivated silicon cluster  $Si_{87}H_{76}$ .

The eigenvalues of the matrix for the left plot of Figure 3.6 are the Chebyshev zeros on  $[-1, 1]$ , i.e.,

$$\lambda_{n-k+1} = \cos\left(\left(k - \frac{1}{2}\right)\frac{\pi}{n}\right), \quad k = 1, 2, \dots, n; \quad n = 10^7. \quad (3.1)$$

It is known that the eigenvalues are clustered at both ends of the interval  $[-1, 1]$ . But our bounds quickly found upper bounds close to 1 within 4 Lanczos steps, with **bnd2** being really sharp even with a small  $k$  such as  $k = 7$ .

The right plot of Figure 3.6 uses a modified matrix: we multiply the smallest 100 eigenvalues from (3.1) by 100 and keep the rest unchanged. Now the eigenvalues are in  $[-100, 1]$ , with the smallest eigenvalues dominating in magnitude and having favorable gaps. Lanczos method should have hard time approximating the largest eigenvalue  $\lambda_n \approx 1$ , relative to converging to the smallest ones. But even for this problem, our bounds still found sharp upper bounds in about 5 steps.

We also implemented the new bounds in the Chebyshev-Davidson algorithm [20]. As expected, a sharper upper bound improves the overall performance of this algorithm. Figure 3.7 contains two typical examples that show the advantage of sharper upper bounds. But we warn that if a bound underestimates the largest eigenvalue, it will result in ineffective Chebyshev filters. In this case unwanted part of spectrum will be magnified instead of dampened, which can lead to very slow convergence or even non-convergence. Appropriate safeguards to ensure upper bounds are essential for constructing effective filters.

## 4 Concluding Remarks

The focus of this note is on cost-effective estimates of an upper bound for the spectrum of large Hermitian matrices. We proposed using very few steps Lanczos iteration with a

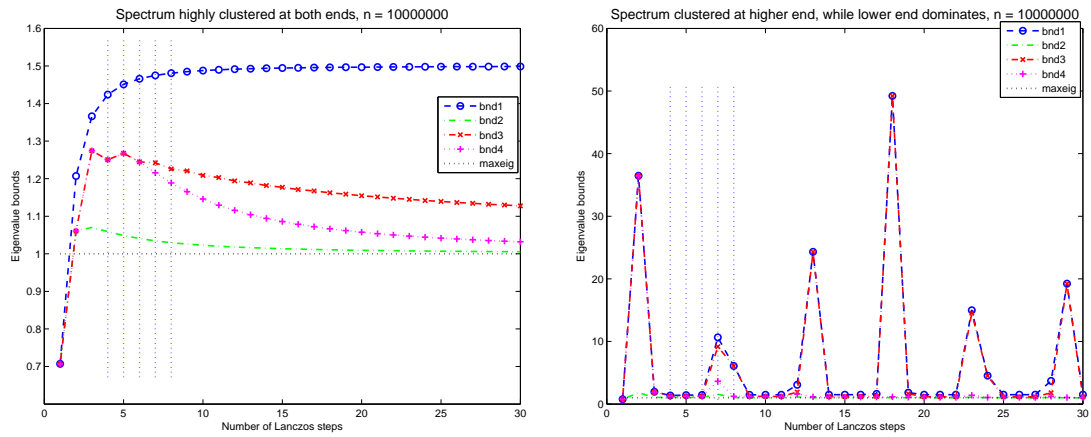


Figure 3.6: Spectrum clustered at both ends. On the right, the smallest eigenvalues dominate in magnitude. From the figure on the right, we again observe that the safeguards for **bnd1** and **bnd3** can be too conservative at certain steps. This again is due to the unbalanced dominance of one end of the spectrum. While **bnd2** provides tight upper bounds consistently with  $k$  increasing.

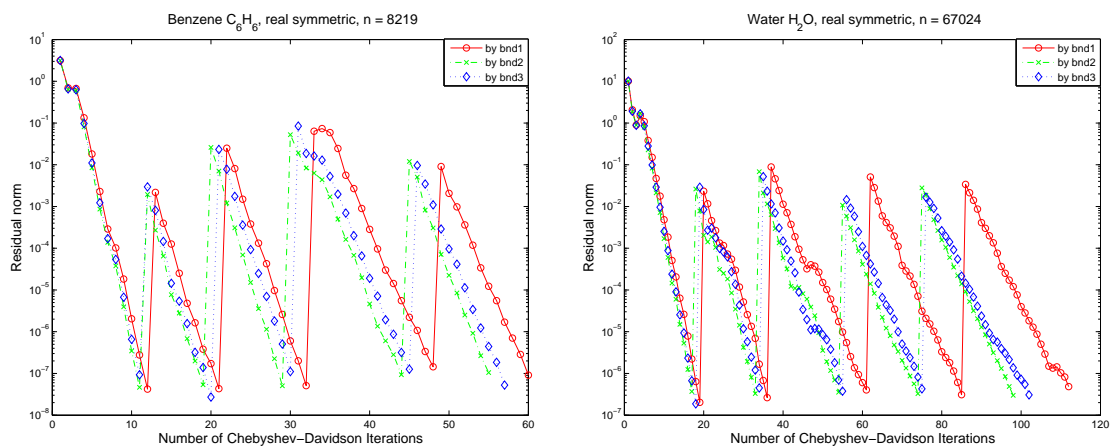


Figure 3.7: Converging 5 eigenvalues and eigenvectors with a relative tolerance of  $1e-7$  using different upper bounds, with all other conditions held the same.

safeguard step. Four closely related bounds are discussed. The safeguards used in the bounds (2.6), (2.8), (2.7), and (2.5) are of increasing strength. A natural question now is: which bound to use in practice? The answer is that it depends. If one can afford a few more Lanczos steps, then (2.6) provides the sharpest upper bound and is preferred. If one is interested in a safe upper bound that can be obtained within as few Lanczos steps as possible, then (2.7) or (2.5) may be the choice. Since the cost for computing all these bounds are similar to computing (2.5), another viable and potentially better choice is to combine some of these bounds. E.g., one can compute (2.6) and (2.7) for a small  $k$  and return the medium of the two as an upper bound; or, one can run a small  $k$  step Lanczos and compute (2.8) at each step, then return the largest one as the upper bound. Notice that hypothesis (2.2) has been the main concern, if in a situation that a vector close to the eigenvector related to  $\lambda_{\max}(A)$  is available, then one can start the Lanczos iteration using this vector instead of a random vector. This will make (2.2) valid in very few Lanczos steps, then (2.6) again becomes the best choice. Such situation exists, for example, when the bound estimator is called within a loop and the previous iteration provides an approximate eigenvector corresponding to the largest eigenvalue.

The bound estimators proposed here can be extended to situations where one needs to estimate extreme singular values through Lanczos bidiagonalization [5, p.495]. One possible application is the computation of (nearly) optimal scaling parameters for calculating the polar factor of a matrix by the scaled Newton iteration [6, p.205].

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