

SOLVING THE REAL EIGENVALUES OF HERMITIAN QUADRATIC EIGENVALUE PROBLEMS VIA BISECTION*

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Abstract. This paper considers solving the real eigenvalues of the Quadratic Eigenvalue Problem (QEP) $Q(\lambda)x \equiv (\lambda^2 M + \lambda C + K)x = 0$ in a given interval (a, b) , where the coefficient matrices M , C , K are Hermitian and M is nonsingular. First, an inertia theorem for the QEP is proven, which characterizes the difference of inertia index between Hermitian matrices $Q(a)$ and $Q(b)$. Several useful corollaries are then obtained, where it is shown that the number of real eigenvalues of QEP $Q(\lambda)x = 0$ in the interval (a, b) is no less than the absolute value of the difference of the negative inertia index between $Q(a)$ and $Q(b)$; furthermore, when all real eigenvalues in (a, b) are semi-simple with the same sign characteristic, the inequality becomes an equality. Based on the established theory, the bisection method (with preprocessing) can be used to compute the real eigenvalues of the QEP by computing the inertia indices. Applications to the calculation of the equi-energy lines with **k.p** model, and also a nonoverdamped mass-spring system are presented in the numerical tests.

Key words. Quadratic eigenvalue problem, Index of inertia, Real eigenvalue, Bisection.

AMS subject classifications. 65F15, 65Z05.

1. Introduction. Let

$$Q(\lambda) := \lambda^2 M + \lambda C + K$$

be a *quadratic matrix polynomial*, where M , C , K are all $n \times n$ complex matrices. The Quadratic Eigenvalue Problem (QEP) is to find scalars λ and nonzero vectors x , $y \in \mathbb{C}^n$ satisfying

$$(1.1) \quad Q(\lambda)x = 0, \quad y^H Q(\lambda) = 0.$$

The scalar λ is called the *eigenvalue* of $Q(\lambda)$, x , y are called the *right and left eigenvectors* of $Q(\lambda)$, respectively, corresponding to λ . QEPs arise in various applications, we refer the readers to a recent survey of QEPs by Tisseur and Meerbergen [29].

In this paper, we consider solving the real eigenvalues of QEPs when all coefficient matrices M , C , K are Hermitian and M is nonsingular. Hereafter, we will call

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QEP with Hermitian coefficient matrices and nonsingular leading coefficient matrix as *Hermitian Quadratic Eigenvalue Problem* (HQEP). Our main thrust of solving real eigenvalues of the HQEP comes from the calculation of the equi-energy lines with the **k.p** model [8], where one needs to solve all positive real eigenvalues of many related medium sized HQEPs to a relative low accuracy, and the number of real eigenvalues is far less than that of the nonreal ones. See a detailed example in Section 4.

The HQEP has $2n$ finite eigenvalues, which are the roots of $\det(Q(\lambda)) = 0$. Though the coefficient matrices M , C , K are all Hermitian, the eigenvalues of the HQEP are in general nonreal, which in nature differs from the case of the linear Hermitian eigenvalue problem, where the eigenvalues must be real. Furthermore, it's easy to see that the nonreal eigenvalues of the HQEP must appear in conjugate pairs, and the number of real eigenvalues, if any, must be even.

The QEPs are usually solved by a two-stage procedure. First, transform the QEP into an equivalent Generalized Eigenvalue Problem (GEP) $Az = \lambda Bz$, where A , B are some $2n$ -by- $2n$ matrices, $z = [x^\top \lambda x^\top]^\top$; second, apply certain numerical methods for the GEP, such as the QZ algorithm [12, 22] for small/medium sized GEPs, and the Krylov subspace based methods for large scale GEPs, such as the Arnoldi method [2] and the two-sided Lanczos method [6]. However, such a procedure suffers from some disadvantages, such as the size of the GEP is twice as large as the original QEP, and more importantly, the structure of the original QEP may not be preserved in the process of linearization. For example, when M , C , K are all positive definite, it's impossible to transform the QEP into a GEP $Az = \lambda Bz$ with A, B Hermitian and B positive definite, i.e., the GEP is intrinsically nonsymmetric. There are also methods that solve the QEP directly without transforming the QEP into a GEP. Such methods usually seek increasingly accurate subspaces, which approximate the subspace spanned by the eigenvectors corresponding to the desired eigenvalues of the QEP, then project the QEP onto the subspaces, and extract the eigen-information of the QEP by solving the reduced order QEP. See for example the residual iteration method [21, 24], the Jacobi-Davidson method for polynomial eigenvalue problem [27], the SOAR method [3],¹ etc.

The main difficulties for solving all real eigenvalues in certain interval (a, b) are twofold. First, computing only partial eigenvalues of the HQEP does not assure one of getting all the real eigenvalues without missing some. One has to develop some technique to check or compute all eigenvalues. Second, it's hard to tell whether the computed eigenvalues close to the real axis are real or not. These two difficulties can be overcome if we could find a method that solves the real eigenvalues of the HQEP like the bisection method that solves the real eigenvalues of a Hermitian/symmetric

¹Though a Companion linearization is implicitly used in SOAR to generate the so called second-order Krylov subspace, we will still say that SOAR solves QEP directly.

matrix, which is based on the Sylvester's law of inertia [7, section 5.3.4]. The inertia theorems for nonlinear eigenvalue problems have been discussed for decades, and recently received a lot of attention, see for example [4, 15, 26] and reference therein. The so called sign characteristic associated with real eigenvalues plays an important role in the spectral analysis for nonlinear eigenvalue problems, which can also be used to discover new inertia results. We refer the readers to the famous GLR theory by I. Gohberg, P. Lancaster and L. Rodman [10, 11] and [16, 17] for more details and further reading. In current literature, inertia theorems are established under proper conditions, which may not hold for general HQEP.

In this paper, with the help of the sign characteristic, we establish an inertia theorem for the HQEP – an equality for the difference of inertia index between Hermitian matrices $Q(a)$ and $Q(b)$. An important inequality is then obtained, which tells that the number of real eigenvalues of HQEP $Q(\lambda)x = 0$ in the interval (a, b) is no less than the absolute value of the difference of the negative inertia index between $Q(a)$ and $Q(b)$. When all real eigenvalues in (a, b) are semi-simple with the same sign characteristic, the inequality becomes an equality. Based on the established theory, a numerical method is proposed, which computes the real eigenvalues of the HQEP via bisection. Compared with other iterative methods, this bisection method is more suitable for computing real eigenvalues, especially when low accuracy is acceptable. Applications to the calculation of the equi-energy lines with the **k.p** model, and a nonoverdamped mass-spring system are presented in the numerical tests, which show that the proposed method is reliable and efficient.

The paper is organized as follows. In Section 2, we establish an inertia theorem for the HQEP. A numerical method based on the established theory is discussed in Section 3. In Section 4, numerical examples are presented, including the calculation of the equi-energy lines with the **k.p** model. Conclusion remarks are given in Section 5.

2. Inertia Theorem for HQEP. In this section, we give an inertia theorem for the HQEP. First, we give the following results on the linearization and spectral decomposition of QEP without proofs. We refer the readers to the GLR theory [10, 11] and [1, 5, 16] for details.

By a special linearization, HQEP (1.1) can be transformed into the following Generalized Eigenvalue Problem (GEP):

$$(2.1) \quad Au = \lambda Bu,$$

where

$$(2.2) \quad A = \begin{bmatrix} -K & 0 \\ 0 & M \end{bmatrix}, \quad B = \begin{bmatrix} C & M \\ M & 0 \end{bmatrix}, \quad u = \begin{bmatrix} x \\ \lambda x \end{bmatrix}.$$

The eigen-information of HQEP (1.1) can be obtained from that of GEP (2.1) and vice versa.

DEFINITION 2.1. [1] A matrix pair $(X, J) \in \mathbb{C}^{n \times 2n} \times \mathbb{C}^{2n \times 2n}$ is called a *standard pair* of the QEP if

1. the matrix $U = U(X, J) := \begin{bmatrix} X \\ XJ \end{bmatrix}$ is nonsingular;
2. $MXJ^2 + CXJ + KX = 0$, or equivalently, $AU = BUJ$.

As a consequence, for a standard pair (X, J) of HQEP (1.1), it holds

$$\lambda(Q) = \lambda(A, B) = \lambda(J),$$

where $\lambda(Q)$, $\lambda(A, B)$ and $\lambda(J)$ are the eigenvalue sets of HQEP (1.1), GEP (2.1) and J , respectively.

Notice that in GEP (2.1), the coefficient matrices A, B are both Hermitian and B is nonsingular and indefinite. Then we can rewrite Theorem 2.2 in [11] as follows:

THEOREM 2.2. *There exists a standard pair (X, J) of HQEP (1.1) such that*

$$\begin{bmatrix} X \\ XJ \end{bmatrix}^H A \begin{bmatrix} X \\ XJ \end{bmatrix} = PJ, \quad \begin{bmatrix} X \\ XJ \end{bmatrix}^H B \begin{bmatrix} X \\ XJ \end{bmatrix} = P,$$

where A, B are defined in (2.2), $J = \text{diag}(\hat{J}_1, \hat{J}_2)$ is the Jordan matrix of $B^{-1}A$ with $\lambda(\hat{J}_1)$ real and $\lambda(\hat{J}_2)$ nonreal, and $P = \text{diag}(\hat{P}_1, \hat{P}_2)$ is a canonical matrix defined by J and sign characteristics. In particular, if J is the following Jordan form

$$J = \text{diag}(\underbrace{J_1, \dots, J_k}_{\hat{J}_1}, \underbrace{J_{k+1}, \bar{J}_{k+1}, \dots, J_{k+\ell}, \bar{J}_{k+\ell}}_{\hat{J}_2}),$$

with $J_i = \text{diag}(J_{i1}, \dots, J_{i, m_i})$, $\lambda(J_i) = \{\lambda_i\}$ for all i , $\lambda_i \neq \lambda_j$ for $i \neq j$, where

$$J_{ij} = \begin{bmatrix} \lambda_i & 1 & & 0 \\ & \lambda_i & 1 & \\ & & \ddots & 1 \\ 0 & & & \lambda_i \end{bmatrix} \in \mathbb{C}^{k_{ij} \times k_{ij}},$$

then

$$(2.3) \quad P = \text{diag} \left(\underbrace{P_1, \dots, P_k}_{\hat{P}_1}, \underbrace{\begin{bmatrix} 0 & P_{k+1} \\ P_{k+1} & 0 \end{bmatrix}, \dots, \begin{bmatrix} 0 & P_{k+\ell} \\ P_{k+\ell} & 0 \end{bmatrix}}_{\hat{P}_2} \right),$$

with

$$\begin{aligned} P_i &= \text{diag}(\epsilon_{i1}P_{i1}, \dots, \epsilon_{i,m_i}P_{i,m_i}), & \text{for } i = 1, \dots, k, \\ P_i &= \text{diag}(P_{i1}, \dots, P_{i,m_i}), & \text{for } i = k+1, \dots, k+\ell, \end{aligned}$$

where $\epsilon_{ij} = \pm 1$,

$$P_{ij} = \begin{bmatrix} 0 & & & 1 \\ & \ddots & & \\ & & 1 & \\ 1 & & & 0 \end{bmatrix} \in \mathbb{C}^{k_{ij} \times k_{ij}}.$$

REMARK 2.3. In Theorem 2.2, the integers m_i, k_{ij} are actually the geometric multiplicity and partial multiplicity of λ_i , respectively. In the diagonal blocks of $\hat{P}_1$ in (2.3), ϵ_{ij} is called the *sign characteristic* [10, 16] of the Hermitian matrix pair (A, B) defined in (2.2).

DEFINITION 2.4. [1, 23] Let λ_i be a real eigenvalue of HQEP (1.1). We call it a real eigenvalue of positive(negative) type if

$$d(x, \lambda_i) = x^H Q'(\lambda_i)x = x^H (C + 2\lambda_i M)x > 0 (< 0),$$

for all x in the null space of $Q(\lambda_i)$. We call it a definite type eigenvalue if it is either of positive type or negative type, a mixed type eigenvalue otherwise.

DEFINITION 2.5. Let λ_i be a real eigenvalue of HQEP (1.1). We say that λ_i has k_+ positive(k_- negative) signs if there exist exactly k_+ (k_-) ϵ_{ij} 's in P_i of $\hat{P}_1$ that are 1(-1).

REMARK 2.6. We can see from Theorem 2.2 that if an eigenvalue $\lambda_i \in \mathbb{R}$ is semi-simple, the corresponding P_{ij} 's are all of order one, consequently, if it is of positive(negative) type, it has m_i positive(negative) signs and zero negative(positive) signs, otherwise λ_i is a mixed type eigenvalue and has a nonzero number of positive and negative signs.

Now we turn to the discussion of the inertia indices of $Q(\sigma)$ and $A - \sigma B$, where A, B are defined in (2.2), $\sigma \in \mathbb{R}$. Hereafter, we will use ' $\sim$ ' to denote the congruence equivalence relation of two matrices, i.e., for any two square matrices Y and Z , we write $Y \sim Z$ if there exists a nonsingular matrix T such that $Y = T^H Z T$. For any Hermitian matrix S , we denote its inertia index by $\text{Inertia}(S) = (\nu(S), \zeta(S), \pi(S))$, where $\nu(S), \zeta(S), \pi(S)$ are the number of negative, zero and positive eigenvalues of S , respectively.

First, we give the following lemma which establishes the relationship between the inertia index of $Q(\sigma)$ and the inertia index of $A - \sigma B$.

LEMMA 2.7. *Let $Q(\lambda)$ be the quadratic matrix polynomial of HQEP (1.1), and let A, B be given by (2.2). Then, for any $\sigma \in \mathbb{R}$, it holds*

$$\text{Inertia}(A - \sigma B) = \text{Inertia}(-Q(\sigma)) + \text{Inertia}(M).$$

Proof. Direct calculation gives rise to

$$\begin{aligned} & \begin{bmatrix} I & 0 \\ \sigma I & I \end{bmatrix}^H (A - \sigma B) \begin{bmatrix} I & 0 \\ \sigma I & I \end{bmatrix} \\ &= \begin{bmatrix} I & 0 \\ \sigma I & I \end{bmatrix}^H \begin{bmatrix} -K - \sigma C & -\sigma M \\ -\sigma M & M \end{bmatrix} \begin{bmatrix} I & 0 \\ \sigma I & I \end{bmatrix} \\ &= \text{diag}(-Q(\sigma), M), \end{aligned}$$

i.e.,

$$A - \sigma B \sim \text{diag}(-Q(\sigma), M),$$

which proves the theorem. $\square$

By Theorem 2.2, we know that

$$A - \sigma B \sim \text{diag}(\widehat{P}_2 \widehat{J}_2 - \sigma \widehat{P}_2, \widehat{P}_1 \widehat{J}_1 - \sigma \widehat{P}_1).$$

Then it follows from the Sylvester law of inertia that

$$(2.4) \quad \text{Inertia}(A - \sigma B) = \text{Inertia}(\widehat{P}_2 \widehat{J}_2 - \sigma \widehat{P}_2) + \text{Inertia}(\widehat{P}_1 \widehat{J}_1 - \sigma \widehat{P}_1).$$

The following lemma tells that the inertia index of $\widehat{P}_2 \widehat{J}_2 - \sigma \widehat{P}_2$ remains unchanged for all $\sigma \in \mathbb{R}$.

LEMMA 2.8. *Let us follow the notation in Theorem 2.2, and let $\text{Inertia}(\widehat{P}_2 \widehat{J}_2 - \sigma \widehat{P}_2) = (\nu_\sigma, \zeta_\sigma, \pi_\sigma)$. Then $\nu_\sigma = \pi_\sigma$, $\zeta_\sigma = 0$ for all $\sigma \in \mathbb{R}$.*

Proof. First, using the fact that $\widehat{P}_2$ is nonsingular and all eigenvalues of $\widehat{J}_2$ are nonreal, we know that $\det(\widehat{P}_2 \widehat{J}_2 - \sigma \widehat{P}_2) = \det(\widehat{P}_2) \det(\widehat{J}_2 - \sigma I) \neq 0$, which implies that $\zeta_\sigma = 0$. Then we only need to show $\nu_\sigma = \pi_\sigma$ for all $\sigma \in \mathbb{R}$.

By Theorem 2.2, we know that

$$\begin{aligned} \widehat{P}_2 \widehat{J}_2 - \sigma \widehat{P}_2 = \text{diag} \left(\begin{bmatrix} 0 & P_{k+1} \bar{J}_{k+1} - \sigma P_{k+1} \\ P_{k+1} J_{k+1} - \sigma P_{k+1} & 0 \end{bmatrix}, \dots, \right. \\ \left. \begin{bmatrix} 0 & P_{k+\ell} \bar{J}_{k+\ell} - \sigma P_{k+\ell} \\ P_{k+\ell} J_{k+\ell} - \sigma P_{k+\ell} & 0 \end{bmatrix} \right). \end{aligned}$$

In the i -th diagonal block of $\widehat{P}_2 \widehat{J}_2 - \sigma \widehat{P}_2$, let the eigenvalue of J_i be $\lambda_i = \alpha_i + \imath \beta_i$ with $\beta_i \neq 0, \imath = \sqrt{-1}$. Then for $i = k+1, \dots, k+\ell$, we have

$$\begin{aligned} & \begin{bmatrix} \imath I & -I \\ \imath I & I \end{bmatrix}^H \begin{bmatrix} 0 & P_i \bar{J}_i - \sigma P_i \\ P_i J_i - \sigma P_i & 0 \end{bmatrix} \begin{bmatrix} \imath I & -I \\ \imath I & I \end{bmatrix} \\ (2.5) \quad &= \begin{bmatrix} P_i(J_i + \bar{J}_i) - 2\sigma P_i & \imath P_i(J_i - \bar{J}_i) \\ \imath P_i(J_i - \bar{J}_i) & -P_i(J_i + \bar{J}_i) + 2\sigma P_i \end{bmatrix} \\ &= \begin{bmatrix} P_i(J_i + \bar{J}_i) - 2\sigma P_i & -2\beta_i P_i \\ -2\beta_i P_i & -P_i(J_i + \bar{J}_i) + 2\sigma P_i \end{bmatrix} := H_i, \end{aligned}$$

where

$$P_i(J_i + \bar{J}_i) - 2\sigma P_i = \text{diag}(\epsilon_{i1} P_{i1}(J_{i1} + \bar{J}_{i1} - 2\sigma I_{k_{i1}}), \dots, \epsilon_{i,m_i} P_{i,m_i}(J_{im_i} + \bar{J}_{im_i} - 2\sigma I_{k_{im_i}})).$$

Now using the structures of J_{ij} and P_{ij} , we have

$$\epsilon_{ij} P_{ij}(J_{ij} + \bar{J}_{ij} - 2\sigma I_{k_{ij}}) = \epsilon_{ij} \begin{bmatrix} 0 & & & 2\alpha_i - 2\sigma \\ & 2\alpha_i - 2\sigma & & 2 \\ & & \ddots & \ddots \\ 2\alpha_i - 2\sigma & 2 & & 0 \end{bmatrix}_{k_{ij} \times k_{ij}},$$

which is a real symmetric matrix. Therefore, H_i defined in (2.5) is a real symmetric Hamiltonian matrix [18, 19, 25], and its positive inertia index is equal to its negative inertia index. Then using

$$\widehat{P}_2 \widehat{J}_2 - \sigma \widehat{P}_2 \sim \text{diag}(H_{k+1}, H_{k+2}, \dots, H_{k+\ell}),$$

we get the conclusion. $\square$

The following lemma will be used to give the inertia index of $\widehat{P}_1 \widehat{J}_1 - \sigma \widehat{P}_1$.

LEMMA 2.9. Let $T_n \in \mathbb{R}^{n \times n}$ be a symmetric matrix given by

$$T_n := \begin{bmatrix} 0 & & & \mu \\ & \mu & & 1 \\ & & \ddots & \ddots \\ \mu & 1 & & 0 \end{bmatrix},$$

where μ is some nonzero real number. Then for $k = 1, 2, \dots$,

$$\text{Inertia}(T_{2k-1}) = \begin{cases} (k-1, 0, k), & \text{if } \mu > 0, \\ (k, 0, k-1), & \text{if } \mu < 0, \end{cases} \quad \text{Inertia}(T_{2k}) = (k, 0, k).$$

Proof. First, it's easy to check that the conclusion holds for $n = 1, 2$. For $n > 2$, we have

$$\begin{aligned} T_n &= \begin{bmatrix} 0 & 0 & \mu \\ 0 & T_{n-2} & e_{n-2} \\ \mu & e_{n-2}^\top & 0 \end{bmatrix} = \begin{bmatrix} 1 & \frac{1}{\mu} & 0 \\ 0 & 1 & 0 \\ 0 & 0 & I_{n-2} \end{bmatrix}^\top \begin{bmatrix} 0 & 0 & \mu \\ 0 & T_{n-2} & 0 \\ \mu & 0 & 0 \end{bmatrix} \begin{bmatrix} 1 & \frac{1}{\mu} & 0 \\ 0 & 1 & 0 \\ 0 & 0 & I_{n-2} \end{bmatrix} \\ &\sim \begin{bmatrix} 0 & 0 & \mu \\ 0 & T_{n-2} & 0 \\ \mu & 0 & 0 \end{bmatrix} \sim \begin{bmatrix} T_{n-2} & 0 & 0 \\ 0 & 0 & \mu \\ 0 & 0 & \mu \end{bmatrix}, \end{aligned}$$

where e_{n-2} is the first column vector of the identity matrix of order $n - 2$. The conclusion follows immediately by mathematical induction. $\square$

Now we are ready to give our main theorem, an inertia theorem for the HQEP.

THEOREM 2.10. *Let $Q(\lambda)$ be the quadratic matrix polynomial of HQEP (1.1). Denote its distinct eigenvalues in (a, b) by $\lambda_1, \lambda_2, \dots, \lambda_r$. Then*

$$(2.6) \quad \nu(Q(a)) - \nu(Q(b)) = \sum_{i=1}^r \sum_{j=1}^{m_i} \epsilon_{ij} \bmod(k_{ij}, 2),$$

where $m_i, \epsilon_{ij}, k_{ij}$ are defined in Theorem 2.2, $\bmod(k_{ij}, 2)$ is the remainder in division of k_{ij} by 2.

Proof. First, using the definition of inertia index and Lemma 2.7, we have

$$\nu(Q(a)) - \nu(Q(b)) = \pi(-Q(a)) - \pi(-Q(b)) = \pi(A - aB) - \pi(A - bB),$$

where A, B are defined in (2.2). Then it follows from (2.4) and Lemma 2.8 that

$$\pi(A - aB) - \pi(A - bB) = \pi(\widehat{P}_1 \widehat{J}_1 - a\widehat{P}_1) - \pi(\widehat{P}_1 \widehat{J}_1 - b\widehat{P}_1),$$

where $\widehat{P}_1, \widehat{J}_1$ are defined in Theorem 2.2. Second, for any $\sigma \in \mathbb{R}$, we have

$$P_{ij}J_{ij} - \sigma P_{ij} = \epsilon_{ij} \begin{bmatrix} 0 & & \lambda_i - \sigma \\ & \lambda_i - \sigma & 1 \\ & \ddots & \ddots \\ \lambda_i - \sigma & 1 & 0 \end{bmatrix} \in \mathbb{R}^{k_{ij} \times k_{ij}},$$

where $J_{ij}, P_{ij}, \epsilon_{ij}, k_{ij}$ are given in Theorem 2.2. Then using Lemma 2.9, for all real eigenvalues outside (a, b) , denoted by $\lambda_{r+1}, \lambda_{r+2}, \dots, \lambda_k$, we know that

$$\pi(P_{ij}J_{ij} - aP_{ij}) - \pi(P_{ij}J_{ij} - bP_{ij}) = 0,$$

for $i = r + 1, r + 2, \dots, k$ and $j = 1, 2, \dots, m_i$. Therefore, it suffices if we can show

$$\pi(P_{ij}J_{ij} - aP_{ij}) - \pi(P_{ij}J_{ij} - bP_{ij}) = \epsilon_{ij} \bmod(k_{ij}, 2),$$

for $i = 1, 2, \dots, r$ and $j = 1, 2, \dots, m_i$. Using Lemma 2.9, we have

$$(2.7) \quad \pi(P_{ij}J_{ij} - aP_{ij}) = \begin{cases} \frac{k_{ij}}{2}, & \text{if } \bmod(k_{ij}, 2) = 0, \\ \frac{k_{ij}+1}{2}, & \text{if } \bmod(k_{ij}, 2) = 1, \epsilon_{ij} = 1, \\ \frac{k_{ij}-1}{2}, & \text{if } \bmod(k_{ij}, 2) = 1, \epsilon_{ij} = -1, \end{cases}$$

and

$$(2.8) \quad \pi(P_{ij}J_{ij} - bP_{ij}) = \begin{cases} \frac{k_{ij}}{2}, & \text{if } \bmod(k_{ij}, 2) = 0, \\ \frac{k_{ij}-1}{2}, & \text{if } \bmod(k_{ij}, 2) = 1, \epsilon_{ij} = 1, \\ \frac{k_{ij}+1}{2}, & \text{if } \bmod(k_{ij}, 2) = 1, \epsilon_{ij} = -1. \end{cases}$$

Combining (2.7) and (2.8), we get

$$\begin{aligned} \pi(P_{ij}J_{ij} - aP_{ij}) - \pi(P_{ij}J_{ij} - bP_{ij}) &= \begin{cases} 0, & \text{if } \bmod(k_{ij}, 2) = 0, \\ 1, & \text{if } \bmod(k_{ij}, 2) = 1, \epsilon_{ij} = 1, \\ -1, & \text{if } \bmod(k_{ij}, 2) = 1, \epsilon_{ij} = -1, \end{cases} \\ &= \epsilon_{ij} \bmod(k_{ij}, 2). \end{aligned}$$

Then the conclusion follows. $\square$

REMARK 2.11. Let us follow the notation in Theorem 2.10. For a real eigenvalue $\lambda_i \in (a, b)$, if

$$\sum_{j=1}^{m_i} \epsilon_{ij} \bmod(k_{ij}, 2) = 0,$$

then λ_i does not make any contribution to the difference between the negative inertia indices, no matter how small the interval is. In such case, this eigenvalue becomes a “ghost”, and can not be detected from the difference between the negative inertia indices.

REMARK 2.12. Let $\lambda = \imath\mu$, Theorem 2.10 can be rewritten as : Let $L(\mu) = \mu^2A + \mu B + C$, where A, C are Hermitian and A is nonsingular, and B is skew-Hermitian. Denote its distinct eigenvalues on the imaginary axis by $\mu_1, \mu_2, \dots, \mu_r$ and $a < \imath\mu_1 < \imath\mu_2 < \dots < \imath\mu_r < b$. Then

$$\nu(L(-\imath a)) - \nu(L(-\imath b)) = \sum_{i=1}^r \sum_{j=1}^{m_i} \epsilon_{ij} \bmod(k_{ij}, 2),$$

where m_i, k_{ij} are the algebraic and partial multiplicities of μ_i , respectively. In such case, the results in [4] can not be applied since $(\hat{K}, \hat{B})$ is not *controllable*, where $\hat{B} = \begin{bmatrix} (B+B^H)/2 \\ 0 \end{bmatrix} = 0$, $\hat{K} = \begin{bmatrix} 0 & -CA^{-1} \\ I & BA^{-1} \end{bmatrix}$.

Theorem 2.10 seems somewhat obscure. What follows will elucidate it with two corollaries.

COROLLARY 2.13. *There exists at least $|\nu(Q(a)) - \nu(Q(b))|$ real eigenvalues of HQEP (1.1) in an interval (a, b) .*

Proof. By Theorem 2.10, we have

$$|\nu(Q(a)) - \nu(Q(b))| \leq \sum_{i=1}^r \sum_{j=1}^{m_i} |\epsilon_{ij}| k_{ij} = \sum_{i=1}^r \sum_{j=1}^{m_i} k_{ij},$$

where the right hand side is exactly the number of real eigenvalues of HQEP (1.1) in (a, b) , counting multiplicities. The conclusion follows. $\square$

Several remarks follow in order.

REMARK 2.14.

1. Let $(a, b) = (0, +\infty)$ and $(a, b) = (-\infty, 0)$, respectively, and note that

$$\text{Inertia}(M) = \text{Inertia}(Q(\pm\infty)), \quad \text{Inertia}(K) = \text{Inertia}(Q(0)).$$

By Corollary 2.13, we can conclude that HQEP (1.1) has at least $2|\nu(M) - \nu(K)|$ real eigenvalues, $|\nu(M) - \nu(K)|$ negative, $|\nu(M) - \nu(K)|$ positive. Notice that the value $|\nu(M) - \nu(K)|$ does not depend on the coefficient matrix C , which enables us to estimate the number of real eigenvalues of HQEP (1.1) from two matrices. This result agrees with the result for the second order equation $m\lambda^2 + c\lambda + k = 0$ with real coefficients: if $|\nu(m) - \nu(k)| = 1$, i.e., $mk < 0$, then $m\lambda^2 + c\lambda + k = 0$ has two real roots, one positive, one negative.

2. Let $a < c < b$ and c is not an eigenvalue of HQEP (1.1), then

$$|\nu(Q(a)) - \nu(Q(b))| \leq |\nu(Q(a)) - \nu(Q(c))| + |\nu(Q(c)) - \nu(Q(b))|,$$

which implies that by dividing the interval into smaller ones, one may find more eigenvalues.

COROLLARY 2.15. *Let us follow the notation in Theorem 2.10. For each eigenvalue $\lambda_i \in (a, b)$, assume that it is semi-simple and has k_i^+ positive signs and k_i^- negative signs. Then*

$$(2.9) \quad \nu(Q(a)) - \nu(Q(b)) = \sum_{i=1}^r (k_i^+ - k_i^-).$$

Furthermore, if all λ_i 's are of the same definite type, then there are $|\nu(Q(a)) - \nu(Q(b))|$ real eigenvalues of HQEP (1.1) in interval (a, b) .

Proof. In Theorem 2.10, let $k_{ij} = 1$ for $i = 1, 2, \dots, r$, $j = 1, 2, \dots, m_i$, then we have

$$\nu(Q(a)) - \nu(Q(b)) = \sum_{i=1}^r \sum_{j=1}^{m_i} \epsilon_{ij} = \sum_{i=1}^r (k_i^+ - k_i^-).$$

When all λ_i 's are of the same definite type, without loss of generality, assume that they are all of positive definite type. Then $\sum_{i=1}^r k_i^- = 0$, and hence,

$$\nu(Q(a)) - \nu(Q(b)) = \sum_{i=1}^r k_i^+,$$

where the number on the right hand side is exactly the number of real eigenvalues of HQEP (1.1) in interval (a, b) . $\square$

Several remarks follow in order.

REMARK 2.16.

1. If a semi-simple real eigenvalue λ_i has the same number of positive and negative signs, then it becomes a "ghost" and can not be detected.
2. For hyperbolic QEP, all eigenvalues are real and semi-simple. Denote the eigenvalues of hyperbolic QEP by $\lambda_1, \lambda_2, \dots, \lambda_{2n}$, in non-increasing order. Using the fact that there exists a $\gamma \in \mathbb{R}$ such that $Q(\gamma)$ is negative definite [20], we know that $\lambda_{2n}, \lambda_{2n-1}, \dots, \lambda_{n+1}$ are all of negative definite type, and $\lambda_n, \lambda_{n-1}, \dots, \lambda_1$ are all of positive definite type. Then it follows from Theorem 2.10 that for any $\sigma > \gamma$, there are $\nu(Q(\sigma)) - \nu(Q(+\infty)) = \nu(Q(\sigma))$ eigenvalues in $(\sigma, +\infty)$, and hence, $2n - \nu(Q(\sigma))$ eigenvalues in $(-\infty, \sigma]$. A similar result can be obtained for $\sigma < \gamma$. These results agree with Theorem 3.1 in [26].

In what follows, we give several small examples to illustrate the above Theorems and Corollaries.

EXAMPLE 2.17. Let

$$M = \begin{bmatrix} -2 & 1 & 0 \\ 1 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}, \quad C = \begin{bmatrix} 5 & -3 & 0 \\ -3 & -2 & 0 \\ 0 & 0 & 0 \end{bmatrix}, \quad K = \begin{bmatrix} -2 & 2 & 0 \\ 2 & 1 & 0 \\ 0 & 0 & -\frac{1}{4} \end{bmatrix}.$$

The eigenvalues of the corresponding HQEP are $-0.5, 0.5, 1$ and 2 . The eigenvalue 1 is of algebraic multiplicity 3 and geometry multiplicity 1, and hence defective. The other three eigenvalues are all simple. Furthermore, the eigenvalues -0.5 and 2 are

of negative type while 1 and 0.5 are of positive type. Therefore, the matrices J and P in Theorem 2.2 can be given by

$$J = \begin{bmatrix} -0.5 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0.5 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 2 \end{bmatrix}, \quad P = \begin{bmatrix} -1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -1 \end{bmatrix}.$$

Now let $(a, b) = (0, 1.5)$. On one hand, by calculation we have $\nu(Q(0)) = 2$, $\nu(Q(1.5)) = 0$ and hence $\nu(Q(0)) - \nu(Q(1.5)) = 2$. On the other hand, the right hand side of equality (2.6) reads

$$1 \times \text{mod}(1, 2) + 1 \times \text{mod}(3, 2) = 1 + 1 = 2.$$

So the equality (2.6) holds, which validates Theorem 2.10.

By Corollary 2.13, we conclude that there exist at least two real eigenvalues in $(0, 1.5)$. However, we don't know whether the two eigenvalues are distinct or not, neither do we know their multiplicities.

EXAMPLE 2.18. Let

$$M = \begin{bmatrix} 2 & 1 \\ 1 & 1 \end{bmatrix}, \quad C = \begin{bmatrix} 4 & 2 \\ 2 & 0 \end{bmatrix}, \quad K = \begin{bmatrix} 2 & 1 \\ 1 & 1 \end{bmatrix}.$$

The eigenvalues of the corresponding HQEP are -1 and 1 . The matrices J and P in Theorem 2.2 can be given by

$$J = \begin{bmatrix} -1 & 1 & & \\ 0 & -1 & & \\ & & 1 & 1 \\ & & 0 & 1 \end{bmatrix}, \quad P = \begin{bmatrix} 0 & 1 & & \\ 1 & 0 & & \\ & & 0 & 1 \\ & & 1 & 0 \end{bmatrix}.$$

In this case, for any $\sigma \in \mathbb{R}/\{-1, 1\}$, we have $\nu(Q(\sigma)) = 2$. Consequently, we can not detect any real eigenvalues by Theorem 2.15. This is because the Jordan blocks of the eigenvalues are all of even order.

EXAMPLE 2.19. Let

$$M = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}, \quad C = \begin{bmatrix} 1 & 0 & 0 \\ 0 & -3 & 0 \\ 0 & 0 & 0 \end{bmatrix}, \quad K = \begin{bmatrix} -2 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & -1 \end{bmatrix}.$$

The eigenvalues of the corresponding HQEP are $-2, -1, 1, 2$. The eigenvalue 1 is semi-simple and has two positive signs and one negative sign, and the other three

eigenvalues $-2, -1, 2$ are all simple and of definite type. The matrices J and P in Theorem 2.2 can be given by

$$J = \text{diag}(-2, -1, 1, 1, 1, 2), \quad P = \text{diag}(-1, -1, 1, -1, 1, 1).$$

Let $(a, b) = (-3, 1.5)$. On one hand, by calculations, we have $\nu(Q(-3)) = 0$, $\nu(Q(1.5)) = 1$. On the other hand, the right hand side of equality (2.9) reads

$$-1 - 1 + (2 - 1) = -1.$$

So the equality (2.9) holds, which validates Corollary 2.15. What's more, according to Corollary 2.13, we can conclude that there exists at least one real eigenvalue in $(-3, 1.5)$. Dividing $(-3, 1.5)$ into $(-3, 0)$ and $(0, 1.5)$, and noticing that $\nu(Q(0)) = \nu(K) = 2$, we know that there exist at least two eigenvalues in $(-3, 0)$ and one eigenvalue in $(0, 1.5)$, i.e., we find more eigenvalues by dividing the interval into smaller ones. However, we can not tell the multiplicity of each eigenvalue.

EXAMPLE 2.20. Let

$$M = \begin{bmatrix} 2 & 0 \\ 0 & 2 \end{bmatrix}, \quad C = \begin{bmatrix} -2 & -2 \\ -2 & -2 \end{bmatrix}, \quad K = \begin{bmatrix} -3 + \varepsilon^2 & 5 + \varepsilon^2 \\ 5 + \varepsilon^2 & -3 + \varepsilon^2 \end{bmatrix}.$$

The eigenvalues of the corresponding HQEP are $-2, 2, 1 \pm \varepsilon i$.

Let $\varepsilon = 10^{-7}$. If we apply the QZ method to the corresponding GEP (2.1), we get the computed eigenvalues $-2.0000, 2.0000, 1.0000 \pm 9.6018 \times 10^{-8}i$. It is hard to tell whether $1.0000 \pm 9.6018 \times 10^{-8}i$ are real eigenvalues or complex ones.

Notice that $\nu(M) = 0$, $\nu(K) = 1$, we conclude that there exists at least one positive eigenvalue and one negative eigenvalue. Now let $(a, b) = (-3, 0)$ in Corollary 2.15, we can use bisection method to find the eigenvalue -2 , and similarly, let $(a, b) = (0, 3)$, we can get the eigenvalue 2 . In such case, the complex eigenvalue pair does not play any role, which is good since we will not mistakenly treat complex eigenvalues as real ones. However, if $\varepsilon = 0$, then the complex eigenvalue pair becomes a real defective eigenvalue 1 with algebraic multiplicity 2 and geometry multiplicity 1 , and hence can not be detected.

3. Numerical method. In this section, we give a numerical method for the HQEP, which computes all/partial real eigenvalues in a given interval.

3.1. Bisection. It follows from Corollary 2.13 that the number of real eigenvalues of HQEP (1.1) in (a, b) is no less than $|\nu(Q(a)) - \nu(Q(b))|$. By Corollary 2.15, if all eigenvalues in (a, b) are semi-simple and of the same definite type, then the number of eigenvalues in (a, b) is exactly $|\nu(Q(a)) - \nu(Q(b))|$. Based on these results, bisection method can be employed to compute the real eigenvalues of HQEP.

First we define the *worklist* as

$$\mathfrak{W} = \{[a, b, n_a, n_b] \mid a < b, n_a = \nu(Q(a)), n_b = \nu(Q(b))\},$$

which contains a list of intervals (a, b) containing at least $|n_a - n_b|$ eigenvalues in it. Then we can present the following bisection algorithm.

ALGORITHM 3.1. *Bisection: This algorithm returns all/partial real eigenvalues in (a, b) to a specified tolerance ε .*

```

W :=  $\emptyset$ ,  $L_{ab} := 0$ 
 $n_a := \nu(Q(a))$ ,  $n_b := \nu(Q(b))$ 
Put  $[a, b, n_a, n_b]$  into W
while W  $\neq \emptyset$ 
    Choose  $a [c, d, n_c, n_d]$  from W and delete it from W
    if  $d - c < \varepsilon$ 
         $L_{ab} = L_{ab} + |n_c - n_d|$ 
        Output: "There are at least  $|n_c - n_d|$  eigenvalues  $\frac{c+d}{2}$  in  $(c, d)$ ."
    else
         $e := \frac{c+d}{2}$ ;  $n_e := \nu(Q(e))$ ,  $n_0 = \zeta(Q(e))$ 
        if  $n_c \neq n_e$  Put  $[c, e, n_c, n_e]$  into W end
        if  $n_e \neq n_d$  Put  $[e, d, n_e, n_d]$  into W end
        if  $n_0 \neq 0$ 
             $L_{ab} = L_{ab} + n_0$ 
            Output: "There are at least  $n_0$  eigenvalues  $e$  in  $(a, b)$ ."
        end
    end
end
Output: " $L_{ab}$  real eigenvalues are detected in  $(a, b)$ ."

```

Several remarks follow.

REMARK 3.1.

1. The integer L_{ab} on output is the number of real eigenvalues detected in (a, b) . And by Corollary 2.13, we know that $L_{ab} \geq |\nu(Q(a)) - \nu(Q(b))|$.
2. The above bisection algorithm is essentially the same as the traditional bisection method that solves all real eigenvalues of a Hermitian/symmetric matrix in a given interval.
3. The eigenvectors corresponding to the computed eigenvalues can be obtained via inverse iteration.
4. The above bisection algorithm for HQEP (1.1) suffers from the following two disadvantages:
 - (a) The efficiency of the algorithm heavily depends on the structure of the

coefficient matrices M, C, K . Unless M, C, K are of a form which enables efficient computation of the inertia of $Q(\sigma)$ for any real parameter σ , the method would be slow.

- (b) If all eigenvalues in (a, b) are semi-simple and of the same sign characteristic, the algorithm returns all real eigenvalues in (a, b) without missing. However, there is no way to find this out prior to calculation.

In order to handle these issues, we need the following preprocessing.

3.2. Preprocessing.

Tridiagonalization. The inertia of a symmetric matrix can be obtained by computing the LDL^T factorization. In the traditional bisection method for a Hermitian/symmetric matrix A , A is first reduced to a tridiagonal matrix T , then for different σ 's, one can obtain the inertia index of $A - \sigma I$ by computing the LDL^T of $T - \sigma I$. For general HQEPs, to tridiagonalize $Q(\sigma)$ for different σ 's via a single congruence transformation, one has to find a matrix W such that $W^H M W$, $W^H C W$ and $W^H K W$ are simultaneously reduced to a tridiagonal form. However, this is in general impossible. We have to find an alternative way to efficiently get the inertias.

According to Lemma 2.7, we know that $\nu(Q(\sigma)) = \pi(A - \sigma B) - \pi(M)$, where A, B are Hermitian matrices defined in (2.2). Then it follows $|\nu(Q(a)) - \nu(Q(b))| = |\pi(A - aB) - \pi(A - bB)|$ for any interval (a, b) . In [28], the author proposed some methods to reduce a symmetric matrix pair (A, B) to a tridiagonal-diagonal matrix pair (T, D) by congruence, where T is tridiagonal, D is diagonal. Therefore, it holds $|\nu(Q(a)) - \nu(Q(b))| = |\nu(T - aD) - \nu(T - bD)|$, and hence, $|\nu(Q(a)) - \nu(Q(b))|$ can be obtained by computing the LDL^T factorizations of two tridiagonal matrices $T - aD$ and $T - bD$, which is quite efficient, though the size of the matrices is doubled.

Counting the number of eigenvalues in (a, b) . If we know the number of real eigenvalues in (a, b) , denoted by N_{ab} , then we can say that Algorithm 3.1 misses $N_{ab} - L_{ab}$ real eigenvalues. In particular, when $L_{ab} = N_{ab}$, Algorithm 3.1 returns all real eigenvalues without missing. Furthermore, if $L_{ab} = N_{ab} = |\nu(Q(a)) - \nu(Q(b))|$, then we can declare that all eigenvalues in (a, b) are semi-simple and of the same sign characteristic. Next we show how to compute the number of eigenvalues in (a, b) with reasonable/affordable cost.

Recall Cauchy's argument principle that the number of zeros of $f(z)$ inside a closed contour $\mathcal{C}$ equals to $\frac{1}{2\pi i} \oint_{\mathcal{C}} \frac{f'(z)}{f(z)} dz$, where $f(z)$ is a meromorphic function inside and on $\mathcal{C}$, and has no zeros on $\mathcal{C}$. Therefore, let $f(\lambda) = \det(Q(\lambda))$ and $\mathcal{C}_{(a,b,\delta)}$ be a rectangular region with four vertexes $a \pm \delta i$, $b \pm \delta i$, where δ is sufficient small enough positive number. If HQEP (1.1) has no eigenvalues on $\mathcal{C}$, then $\frac{1}{2\pi i} \oint_{\mathcal{C}_{(a,b,\delta)}} \frac{f'(z)}{f(z)} dz$ is the number of eigenvalues in $\mathcal{C}_{(a,b,\delta)}$, which can be used to estimate N_{ab} .

The value of $\frac{1}{2\pi i} \oint_C \frac{f'(z)}{f(z)} dz$ can be evaluated via some numerical integration algorithms, for example the adaptive Simpson quadrature. First we reduce (A, B) to (T, D) by congruence via tridiagonalization. Then using

$$\det(A - \lambda B) = (-1)^n \det(M) \det(Q(\lambda))$$

and the Jacobi's formula, we can show that the values of $\frac{f'(z)}{f(z)}$ at certain point z_0 , which is repeatedly used in numerical integration, can be given by

$$\frac{f'(z_0)}{f(z_0)} = \frac{\det'(A - z_0 B)}{\det(A - z_0 B)} = -\text{trace}((A - z_0 B)^{-1} B) = -\text{trace}((T - z_0 D)^{-1} D).$$

In [26], an efficient and stable $\mathcal{O}(n)$ algorithm is provided to compute $\text{trace}(T_1^{-1} T_2)$ for tridiagonal matrices T_1, T_2 , which enables us to efficiently compute $\frac{f'(z_0)}{f(z_0)} = -\text{trace}((T - z_0 D)^{-1} D)$.

Several remarks follows.

REMARK 3.2.

1. How to choose δ and the tolerance τ of the numerical integration can be tricky. A too small δ will lead to oscillation in $\frac{f'(z)}{f(z)}$, and hence requires a small τ , which can be quite expensive; a large δ will increase the possibility that the unwanted complex eigenvalues drop into $\mathcal{C}_{(a,b,\delta)}$. In our numerical tests, we will simply set $\delta = 4 \times 10^{-4}$, $\tau = 0.05$.
2. Counting the number of eigenvalues in (a, b) based on Cauchy's argument principle can also be treated as a general method to compute eigenvalues in (a, b) . But its disadvantages are obvious. First, we still could not tell whether the computed eigenvalues, which are close to real axis, are real or not; second, δ and τ are difficult to choose; third, comparing with the bisection method, it can be much more expensive. One may resolve these issues with more detailed works, but we will not treat these issues in this paper.

With the above preprocessing (performed only once), we can estimate the number of real eigenvalues in (a, b) by $N_{ab} \approx \frac{1}{2\pi i} \oint_C \frac{f'(z)}{f(z)} dz$. Then if $N_{ab} \neq 0$, we can use Algorithm 3.1 to compute real eigenvalues of HQEP, and the last line of Algorithm 3.1 can be replaced by

Output: “ L_{ab} real eigenvalues are detected in (a, b) , $N_{ab} - L_{ab}$ are missing.”

4. Numerical tests. In this section, we apply Algorithm 3.1 to compute the real eigenvalues of some structured HQEPs. Two numerical tests are presented: the first one is a block tridiagonal HQEP, which comes from the calculation of the equi-energy lines with the **k.p** model [8]; the second is a tridiagonal HQEP, which comes from a nonoverdamped mass-spring system. All numerical tests are carried out on an

Intel(R) Core(TM)i7 2.30GHz processor with 8.0GB RAM, using MATLAB 2012a. We will compare Algorithm 3.1 with the ‘quadeig’ function in [13], the MATLAB function ‘polyeig’ and shift-invert SOAR method in [3] in two aspects: CPU time and accuracy of the computed eigenvalue. The accuracy of the computed eigenvalue $\hat{\lambda}$ is measured by the relative error

$$\frac{|\hat{\lambda} - \lambda|}{|\lambda|},$$

where λ is the exact eigenvalue, or the relative residual

$$\frac{\|Q(\hat{\lambda})\hat{x}\|_1}{(|\hat{\lambda}|^2\|M\|_1 + |\hat{\lambda}|\|C\|_1 + \|K\|_1)\|\hat{x}\|_1},$$

where $\hat{x}$ is the approximated eigenvector obtained via the inverse iteration of $Q(\hat{\lambda})$. As the exact eigenvalue is not available in general, we will use the computed eigenvalue from Algorithm 3.1 as the “exact” one since it could solve the eigenvalue to any precision.

4.1. Calculation of the equi-energy lines with the $\mathbf{k.p}$ model. In order to understand and predict the electronic properties of a material, one usually needs to know the band structure of it first. One of the widely used methods to determine the band structure is the $\mathbf{k.p}$ method, which is based on the discretization of the Schrödinger equation and is well suited to determine the band structure of silicon and germanium, in the absence of spin-orbit coupling. An algebraic eigenvalue problem can be derived from the $\mathbf{k.p}$ model, where in order to calculate the equi-energy lines, one needs to solve the magnitude of the wave-vector, in a given direction and certain energy E . In the 2D case, from the 6×6 $\mathbf{k.p}$ model, a quadratic eigenvalue problem can be obtained by means of finite differences with a uniform mesh. The quadratic eigenvalue problem can be given by

$$(4.1) \quad H(k)\xi_k = [k^2 H_2 + k H_1 + (H_0 - EI)]\xi_k = 0,$$

where k is the magnitude of the wave-vector, θ is the angle, E is the energy, ξ_k is a vector of length $6N_z$ (N_z is the number of discretization points). The matrices

H_2, H_1, H_0 can be given by

$$H_2 = \begin{bmatrix} H_2^d(\theta) & & & 0 \\ & H_2^d(\theta) & & \\ & & \ddots & \\ 0 & & & H_2^d(\theta) \end{bmatrix}, \quad H_1 = \begin{bmatrix} 0 & H_1^+(\theta) & & & 0 \\ -H_1^+(\theta) & 0 & H_1^+(\theta) & & \\ & \ddots & \ddots & \ddots & \\ 0 & & & \ddots & H_1^+(\theta) \\ & & & -H_1^+(\theta) & 0 \end{bmatrix},$$

$$H_0 = \begin{bmatrix} H_0^d + D_1 I & H_0^+ & & & \\ H_0^+ & H_0^d + D_2 I & H_0^+ & & \\ & \ddots & \ddots & \ddots & \\ & & \ddots & H_0^d + D_{N_z-1} I & H_0^+ \\ 0 & & & H_0^+ & H_0^d + D_{N_z} I \end{bmatrix},$$

where $H_2^d(\theta)$, H_0^d , $H_0^+(\theta)$ are all 6×6 Hermitian matrices with $H_2^d(\theta)$ negative definite. $H_1^+(\theta)$ is a 6×6 skew-Hermitian matrix and $D_i I$ is a scalar matrix for $i = 1, \dots, N_z$. Consequently, H_2, H_1, H_0 are all Hermitian and block tridiagonal matrices. For any given energy E for angle θ , we need to compute all real positive eigenvalues of (4.1). We refer the readers to [8] for more details on the **k.p** model and how the above QEP is formulated.

As the order of magnitudes of H_2, H_1, H_0 are dramatically different, we use the parameter scaling [9] and set $Q(\lambda) = \frac{1}{\beta} H(\alpha\lambda) = \lambda^2 M + \lambda C + K$, where

$$M = \frac{\alpha^2}{\beta} H_2, \quad C = \frac{\alpha}{\beta} H_1, \quad K = \frac{1}{\beta} (H_0 - EI),$$

α, β are two parameters. Then we can obtain the eigenvalues of $H(k)$ via $Q(\lambda)$, whose the positive eigenvalues are the ones of interest.

For silicon, all positive real eigenvalues of $Q(\lambda) = \lambda^2 M + \lambda C + K$ are semi-simple and of negative type, which enables us to compute all real positive eigenvalues by Algorithm 3.1. What's more, notice that for any $\sigma \in \mathbb{R}$, $Q(\sigma)$ is a block tridiagonal matrix. Therefore, we can efficiently obtain the inertia index of $Q(\sigma)$ by the block LDL^T factorization of it.

Now let $N_z = 250$, then M, C, K are of order 1500. Fix the angle $\theta = \frac{\pi}{2}$. We set $(a, b) = (0, 0.1)$, ² $\varepsilon = 10^{-13}$ in Algorithm 3.1 so that the relative error and relative residual are of the same order of magnitude with 'polyeig' and 'quadeig'. For different energy E , we list the relative errors, relative residuals and CPU times for Algorithm 3.1 (bisection), 'quadeig' and 'polyeig' in Table 4.1.

²The upper bound for all positive real eigenvalues can be obtained via techniques developed in [14].

E	L_{ab}	bisection	quadeig	polyeig	SOAR
max relative error					
-2.0	26		4.74e-12	3.23e-11	8.01e-07
-1.6	20		6.83e-12	9.12e-12	5.51e-07
-1.2	18		6.61e-12	3.71e-11	1.41e-08
-0.8	14		3.28e-12	2.30e-11	4.02e-11
-0.4	10		4.22e-12	4.59e-11	3.92e-12
max relative residual					
-2.0	26	9.16e-14	6.32e-14	8.14e-14	1.22e-06
-1.6	20	4.22e-14	2.78e-14	9.06e-14	1.40e-07
-1.2	18	1.49e-14	5.67e-14	9.13e-14	2.18e-07
-0.8	14	8.00e-14	9.58e-14	1.27e-14	3.07e-09
-0.4	10	4.85e-14	1.58e-14	9.04e-14	1.68e-11
time in seconds					
-2.0	26	22.92	1491	2092	24.58
-1.6	20	17.58	1465	2082	19.12
-1.2	18	14.47	1479	2011	15.86
-0.8	14	11.43	1460	2126	11.65
-0.4	10	9.001	1475	2178	8.471

TABLE 4.1
Accuracy and CPU time for the **k.p** model test.

We can see from Table 4.1 that as the energy E increases from -2.0 to -0.4 , the number of positive real eigenvalues L_{ab} decreases from 26 to 10. Compared with ‘quadeig’ and ‘polyeig’, bisection wins a little bit in accuracy and with much less CPU time. This is due to the fact that bisection only needs to compute a few positive real eigenvalues, while ‘quadeig’ and ‘polyeig’ have to compute all eigenvalues to full precision in order to find all positive real eigenvalues. As a matter of fact, in practical applications, one only needs to solve the eigenvalues to a low precision, say 5 or 6 significant digits. In such case, bisection saves more CPU time, while ‘quadeig’ and ‘polyeig’ still need to compute to full precision.

The CPU time listed for SOAR is obtained by solving the eigenvalues with largest magnitude from $(\mu^2 K + \mu C + M)x = 0$, where $\mu = 1/\lambda$. In such case, real eigenvalues in SOAR converge faster as the real eigenvalues are among the ones with largest magnitude. However, if we perform SOAR (with shift-invert) to the original $Q(\lambda)$, SOAR is not able to find all real eigenvalues with a single shift.

4.2. A nonoverdamped mass-spring system. Now we consider a tridiagonal HQEP

$$Q(\lambda) = \lambda^2 M + \lambda C + K,$$

where

$$M = I_n, \quad C = \tau \operatorname{tridiag}(-1, 3, -1), \quad K = \kappa \operatorname{tridiag}(-1, 3, -1).$$

This HQEP comes from the nonoverdamped mass-spring system [29]. We take $n = 1000$ and choose $\tau = 0.6202$, $\kappa = 0.4807$. The distribution of eigenvalues is plotted in Figure 4.1, and all 20 real eigenvalues are listed below, which are quite clustered.

$\lambda_1 = -1.57385316529652,$	$\lambda_2 = -1.57353777489852,$
$\lambda_3 = -1.57300288871881,$	$\lambda_4 = -1.57223325936736,$
$\lambda_5 = -1.57120423100026,$	$\lambda_6 = -1.56987682525908,$
$\lambda_7 = -1.56818760580577,$	$\lambda_8 = -1.56602506425224,$
$\lambda_9 = -1.56316146756131,$	$\lambda_{10} = -1.55895134438424,$
$\lambda_{11} = -1.54143781528440,$	$\lambda_{12} = -1.53734374405367,$
$\lambda_{13} = -1.53458398638326,$	$\lambda_{14} = -1.53251306990164,$
$\lambda_{15} = -1.53090326066911,$	$\lambda_{16} = -1.52964304951539,$
$\lambda_{17} = -1.52866899944061,$	$\lambda_{18} = -1.52794213154477,$
$\lambda_{19} = -1.52743778956278,$	$\lambda_{20} = -1.52714072580375.$

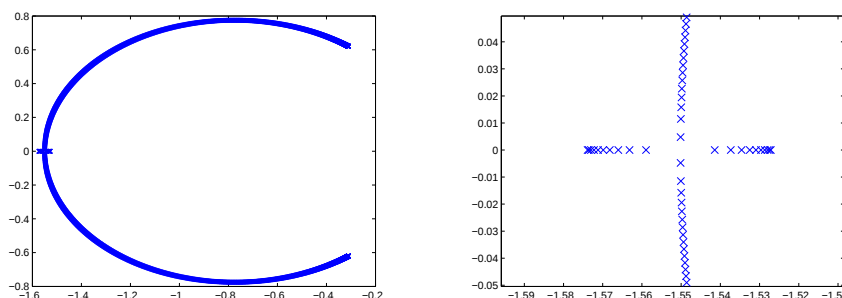


FIG. 4.1. *Eigenvalue distribution (left: all eigenvalues, right: real eigenvalues).*

The smaller ten real eigenvalues are of negative type and the larger ten are of positive type. For different intervals, we use Algorithm 3.1 (with preprocessing) to compute all twenty real eigenvalues, where the tolerance ε is set to be 10^{-11} . The numerical results are listed in Table 4.2, from which we can see that the number of

real eigenvalues detected by Algorithm 3.1 can be quite sensitive for different choices of intervals. This is because all twenty real eigenvalues in this example are clustered, and the sum of the sign characteristics of all twenty eigenvalues is zero.

Interval (a, b)	L_{ab}	$N_{ab} - L_{ab}$
$(-1.6000, -1.5000)$	20	0
$(-1.6219, -1.5073)$	16	4
$(-1.6437, -1.4944)$	12	8
$(-1.6568, -1.4866)$	8	12
$(-1.6644, -1.4821)$	4	16

TABLE 4.2

Number of detected and missing eigenvalues vs. different intervals.

In the following tests, we choose the interval $(a, b) = (-1.6, -1.5)$. The numerical integral for $\frac{1}{2\pi i} \oint_C \frac{f'(z)}{f(z)} dz$ in the preprocessing is computed by the MATLAB function ‘quad’, and it costs 17.7841 CPU time (in seconds).

In Table 4.3, we compare bisection with ‘quadeig’ and ‘polyeig’ in accuracy and CPU time, which again shows that bisection is as accurate as ‘quadeig’ and ‘polyeig’, much more efficient, even with affordable preprocessing.

	bisection	quadeig	polyeig
CPU Time	11.85	124.9	219.6
max relative residual	4.24e-14	1.98e-14	5.67e-14
max relative error		3.25e-13	6.03e-13

TABLE 4.3

Accuracy and CPU time.

In Table 4.4, we list the numerical results for (shift-invert) SOAR with different shifts and search space sizes, the integer in parentheses after the shift stands for the search space size. SOAR with the mid-point of $(-1.6, -1.5)$ as the shift and relative large search space size 400, fails to give any real eigenvalues. While if we take -1.575 as the shift, and 100 and 400 as the search space sizes, respectively, SOAR returns better results. However, it is hard to choose proper shift and search space size prior to calculation. Of course, one can continue to pursue SOAR with multiple shifts, but inevitably, one needs to choose proper shifts.

5. Conclusion. In this paper, we considered solving real eigenvalues of HQEP $Q(\lambda)x = (\lambda^2 M + \lambda C + K)x = 0$ in an interval (a, b) . An inertia theorem for the HQEP is given, which characterizes the difference of inertia index between $Q(a)$ and $Q(b)$. Two useful corollaries are then obtained: the number of real eigenvalues of the HQEP in the interval (a, b) is no less than the absolute value of the difference

shift(search space size)	-1.575(400)	-1.550(400)	-1.575(100)
CPU Time	8.206	7.129	2.558
max relative residual	1.35e-12	1.145	4.27e-04
max relative error	1.98e-11	0.076	5.91e-05

TABLE 4.4

Accuracy and CPU time of SOAR with different shifts and search space sizes.

of the negative inertia index between $Q(a)$ and $Q(b)$; when all real eigenvalues in (a, b) are semi-simple and of the same definite type, the number of real eigenvalues in (a, b) is exactly the absolute value of the difference of the negative inertia index between $Q(a)$ and $Q(b)$. Based on the established theory, bisection method (with preprocessing) can be used to compute all/partial real eigenvalues of the HQEP. This method is able to find all real eigenvalues in given interval when all real eigenvalues in the interval are semi-simple and of the same definite type. Furthermore, compared with other iterative methods, this proposed method is more suitable for computing real eigenvalues, especially when low accuracy is acceptable. Numerical tests show that this method is reliable and efficient. Lastly, it is worth mentioning here that the theorem and corollaries in this paper can be generalized to Hermitian matrix polynomials of higher order.

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