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# THE RADAU–LANCZOS METHOD FOR MATRIX FUNCTIONS*

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**Abstract.** Analysis and development of restarted Krylov subspace methods for computing $f(A)\boldsymbol{b}$ have proliferated in recent years. We present an acceleration technique for such methods when applied to Stieltjes functions $f$ and Hermitian positive definite matrices $A$. This technique is based on a rank-one modification of the Lanczos matrix derived from a connection between the Lanczos process and Gauss–Radau quadrature. We henceforth refer to the technique paired with the standard Lanczos method for matrix functions as the Radau–Lanczos method for matrix functions. We develop properties of general rank-one updates, leading to a framework through which other such updates could be explored in the future. We also prove error bounds for the Radau–Lanczos method, which are used to prove the convergence of restarted versions. We further present a thorough investigation of the Radau–Lanczos method explaining why it routinely improves over the standard Lanczos method. This is confirmed by several numerical experiments, and we conclude that, in practical situations, the Radau–Lanczos method is superior in terms of iteration counts and timings, when compared to the standard Lanczos method.

**Key words.** matrix functions, Krylov subspace methods, restarted Lanczos method, Gaussian quadrature, Gauss–Radau quadrature

**AMS subject classifications.** 65F60, 65F50, 65F10, 65F30

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## 1. Introduction.

A problem of increasing importance in scientific computing is the computation of $f(A)\boldsymbol{b}$, where $f$ is a scalar function, $A \in \mathbb{C}^{n\times n}$, and $\boldsymbol{b} \in \mathbb{C}^n$. Frequently $A$ is large and sparse, making the direct computation of $f(A)$ infeasible, but not $f(A)\boldsymbol{b}$. Applications requiring $f(A)\boldsymbol{b}$ include the solution of differential equations via exponential integrators [18, 19, 20]; determining the communicability—or other quantities of interest—in network analysis [2, 8]; and simulations involving the Neuberger overlap operator or the rational hybrid Monte Carlo algorithm in lattice quantum chromodynamics [3, 7].

In practice, $f(A)\boldsymbol{b}$ is often approximated using a Krylov subspace method. While such methods are effective, computer memory can limit the number of iterations that can be performed—and thus the attainable accuracy—as the entire Krylov basis must be stored. A typical remedy for this problem is the use of *restarted* Krylov subspace methods [1, 5, 9, 10, 21], in which the current error is expressed in the form $e(A)\boldsymbol{v}$ with a new matrix function $e$ and a vector $\boldsymbol{v}$ from the previous Krylov space. Using divided differences to evaluate $e$ as is done in [21] tends to introduce numerical instabilities, which is why the other references use alternative ways to evaluate $e$—particularly

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integral representations—which perform in a numerically stable manner. While effective in overcoming the storage problem, restarts typically require more iterations, and therefore more time, to converge to the desired accuracy. Therefore, cheap modifications that accelerate convergence with restarts without increasing computational effort are attractive from a practitioner's point of view. One modification used for this purpose is the *deflated restarting technique*, as in [6], which can in some cases accelerate convergence by using Ritz value information to implicitly deflate certain eigenvectors of the problem matrix. The main contribution of this paper is another such modification, which we call the (restarted) Radau–Lanczos method for computing $f(A)\boldsymbol{b}$. We prove error bounds for the unrestarted Radau–Lanczos method, which are used to show that the restarted Radau–Lanczos method converges when $A$ is Hermitian positive definite (HPD) and $f$ is a Stieltjes function. With practical numerical experiments, we demonstrate that the modified method routinely improves over the standard method in terms of iteration counts and execution times, especially in situations where the Ritz values generated by the restarted Lanczos method poorly approximate the extremal eigenvalues of $A$.

An outline of the paper is as follows. We begin by establishing properties of the standard Lanczos method and of the Lanczos relation. In section 2, we describe the Radau–Lanczos method for linear systems, including a variational characterization that yields error bounds similar to those of the conjugate gradient (CG) method. This analysis serves as a necessary building block in developing the Radau–Lanczos approach for matrix functions. In section 3, we apply the Radau–Lanczos method to Stieltjes functions of HPD matrices and show that the restarted version converges by providing convergence bounds. In the subsequent sections, we perform various numerical experiments in order to illustrate important features of our method. The experiments of section 4 investigate and compare the interpolating polynomials implicitly generated by the standard Lanczos method and the Radau–Lanczos method. These experiments help us gain some insight into why the proposed method is superior. In section 5, we further compare both methods via several model problems from applications in scientific computing. Concluding remarks are given in section 6.

**1.1. The standard Lanczos method.** We begin by recalling the essentials of the standard Lanczos approach for $A \in \mathbb{C}^{n\times n}$ HPD and $f(z) = z^{-1}$, resulting in the CG method for linear systems; see, e.g., [26]. Consider the linear system

$$A\boldsymbol{x} = \boldsymbol{b}. \tag{1}$$

Let $\boldsymbol{x}_*$ be the exact solution to (1); $\boldsymbol{x}_0$ the starting approximation; $\boldsymbol{x}_m$ the iterates; $\boldsymbol{e}_m = \boldsymbol{x}_* - \boldsymbol{x}_m$ the errors; and $\boldsymbol{r}_m = A\boldsymbol{e}_m = \boldsymbol{b} - A\boldsymbol{x}_m$ the residuals. We also let $\mathcal{K}_m(A, \boldsymbol{r}_0)$ denote the $m$th Krylov subspace corresponding to $A$ and the initial residual $\boldsymbol{r}_0 \neq \boldsymbol{0}$, and $\Pi_m$ the space of all polynomials of degree at most $m$. Then $\mathcal{K}_m(A, \boldsymbol{r}_0) = \{p(A)\boldsymbol{r}_0 : p \in \Pi_{m-1}\}$. We refer to the following as the *Lanczos relation*:

$$AV_m = V_m T_m + t_{m+1,m}\boldsymbol{v}_{m+1}\widehat{\boldsymbol{e}}_m^H, \tag{2}$$

where the columns of $V_m \in \mathbb{C}^{n\times m}$ form an orthonormal basis of $\mathcal{K}_m(A, \boldsymbol{r}_0)$; $T_m = V_m^H A V_m \in \mathbb{C}^{m\times m}$ is the restriction and projection of $A$ onto $\mathcal{K}_m(A, \boldsymbol{r}_0)$; and $\widehat{\boldsymbol{e}}_m$ is the $m$th standard unit vector with appropriate dimension. Since $A$ is Hermitian, $T_m$ is tridiagonal and real. The matrices $V_m$ and $T_m$ expand from those with smaller indices as follows:

$$V_{m+1} = [V_m \mid \boldsymbol{v}_{m+1}], \;\; T_{m+1} = \begin{bmatrix} T_m & t_{m+1,m}\widehat{\boldsymbol{e}}_m \\ \widehat{\boldsymbol{e}}_m^H t_{m+1,m} & t_{m+1,m+1} \end{bmatrix}.$$

Moreover, all entries $t_{m+1,m}$ are nonzero up to some index $m = \mathrm{gr}_A(\boldsymbol{r}_0)$, the *grade* of $\boldsymbol{r}_0$ with respect to $A$, i.e., the first index $m$ for which $\mathcal{K}_{m+1}(A, \boldsymbol{r}_0) = \mathcal{K}_m(A, \boldsymbol{r}_0)$. The Lanczos relation (2) thus holds up to precisely $m = \mathrm{gr}_A(\boldsymbol{r}_0)$ with $\boldsymbol{v}_{m+1} = \boldsymbol{0}$.

Mathematically, the $m$th iterate $\boldsymbol{x}_m$ of CG or, equivalently, the Lanczos method, is given as follows:

$$\boldsymbol{x}_m = \boldsymbol{x}_0 + V_m T_m^{-1} V_m^H \boldsymbol{r}_0 = \boldsymbol{x}_0 + V_m q_{m-1}(T_m) V_m^H \boldsymbol{r}_0,$$

where $q_{m-1} \in \Pi_{m-1}$ is the polynomial interpolating $f(z) = z^{-1}$ at the eigenvalues of $T_m$. Indeed, $T_m^{-1} = q_{m-1}(T_m)$; see, e.g., [17, Chap. 1].

We also know that $\boldsymbol{x}_m = \boldsymbol{x}_0 + p(A)\boldsymbol{r}_0$ for some polynomial $p \in \Pi_{m-1}$. The fact that $\boldsymbol{x}_m$ has a unique representation in $\boldsymbol{x}_0 + \mathcal{K}_m(A, \boldsymbol{r}_0)$, plus the following lemma [25, Lemma 3.1], ensures that $p$ and $q_{m-1}$ are, in fact, the same.

LEMMA 1.1 (Lanczos polynomial relation). *For all $q \in \Pi_{m-1}$,*

$$V_m q(T_m) V_m^H \boldsymbol{r}_0 = q(A)\boldsymbol{r}_0. \tag{3}$$

Since $A$ is HPD, the following is an inner product $(\cdot,\cdot)$ on $\Pi_m$ as long as $m \leq \mathrm{gr}_A(\boldsymbol{r}_0)$:

$$(p, q) := \langle p(A)\boldsymbol{r}_0, q(A)\boldsymbol{r}_0 \rangle_2 = (p(A)\boldsymbol{r}_0)^H q(A)\boldsymbol{r}_0,$$

where $\langle\cdot,\cdot\rangle_2$ denotes the usual Euclidean inner product. Expanding $\boldsymbol{r}_0 = \sum_{i=1}^n \beta_i \boldsymbol{u}_i$ in terms of an orthonormal basis of $\mathbb{C}^n$ consisting of eigenvectors $\boldsymbol{u}_i$ of $A$ with corresponding eigenvalues $\lambda_i$, we can express this inner product as

$$(p, q) = \sum_{i=1}^n |\beta_i|^2 \bar{p}(\lambda_i) q(\lambda_i) = \int_{\lambda_{\min}}^{\lambda_{\max}} \bar{p}(z) q(z) \, \mathrm{d}\alpha(z).$$

Here $\lambda_{\min}$ and $\lambda_{\max}$ denote the smallest and largest eigenvalue of $A$, respectively, and the measure $\mathrm{d}\alpha$ is defined by the function $\alpha(z) = \sum_{i=1}^n |\beta_i|^2 H(z - \lambda_i)$ with $H$ denoting the Heaviside function.

If $p$ is a polynomial with $p(0) \neq 0$, then we denote $\widetilde{p} = \frac{1}{p(0)} p$ as its normalized variant, so that $\widetilde{p}(0) = 1$. We denote by $p_m$ the sequence of orthogonal polynomials with respect to $(\cdot,\cdot)$. It is known that the zeros of $p_m$ are the eigenvalues of $T_m$, as well as the nodes of the $m$-point Gauss quadrature rule with respect to $\mathrm{d}\alpha$ on $[\lambda_{\min}, \lambda_{\max}]$; see [13, 14]. These orthogonal polynomials are unique up to a scaling factor, and we call the corresponding normalized $\widetilde{p}_m$ the CG polynomials because of the following well-known result; see, e.g., [23, Chap. 8], where $\|\boldsymbol{v}\|_A$ denotes the *energy norm* of a vector $\boldsymbol{v}$, induced by the inner product $\langle \boldsymbol{v}, \boldsymbol{w} \rangle_A := \boldsymbol{v}^H A \boldsymbol{w}$.

THEOREM 1.2. *The CG iterates $\boldsymbol{x}_m$ satisfy*

(i) $\boldsymbol{e}_m = \widetilde{p}_m(A)\boldsymbol{e}_0$, $\boldsymbol{r}_m = \widetilde{p}_m(A)\boldsymbol{r}_0$;

(ii) $\|\boldsymbol{e}_m\|_A = \min\{\|\boldsymbol{x}_* - \boldsymbol{x}\|_A : \boldsymbol{x} \in \boldsymbol{x}_0 + \mathcal{K}_m(A, \boldsymbol{r}_0)\}$.

In subsequent results, we will require energy norms for functions of HPD matrices $A$. For functions $g : (0, \infty) \to (0, \infty)$, the matrix $g(A)$ is HPD when $A$ is HPD. Then the inner product

$$\langle \boldsymbol{x}, \boldsymbol{y} \rangle_{g(A)} := \langle \boldsymbol{x}, g(A)\boldsymbol{y} \rangle \quad \text{for all} \quad \boldsymbol{x}, \boldsymbol{y} \in \mathbb{C},$$

induces the norm

$$\|\boldsymbol{x}\|_{g(A)} := \langle \boldsymbol{x}, \boldsymbol{x} \rangle_{g(A)}.$$

**1.2. Rank-one modifications.** In [9], the authors consider a particular rank-one modification of the matrix $T_m$ for computing approximations to $f(A)\boldsymbol{b}$. This modification serves two purposes. First, it broadens the class of matrices for which convergence of the restarted Arnoldi method can be proven to include non-Hermitian positive real matrices (i.e., matrices with field of values in the right half-plane). Second, as illustrated by numerical experiments in [9], it sometimes converges faster than the standard restarted Arnoldi method, especially for severely non-Hermitian matrices. This modified method, called the *harmonic Arnoldi method*, is based on the Arnoldi relation rather than the Lanczos relation (2), because it is mainly designed for non-Hermitian matrices. We briefly recapitulate how the modification works for $A$ HPD (which is also positive real). to serve as motivation for our new method, and we prove general results about rank-one modifications of the Lanczos relation.

Define $\widetilde{T}_m := T_m + \big(t_{m+1,m}T_m^{-1}\widehat{\boldsymbol{e}}_m\big)\widehat{\boldsymbol{e}}_m^H$ and the corresponding iterates

$$\widetilde{\boldsymbol{x}}_m := \boldsymbol{x}_0 + V_m\widetilde{T}_m^{-1}V_m^H\boldsymbol{r}_0.$$

By the following lemma we can conclude, just as with CG, that

$$\widetilde{\boldsymbol{x}}_m = \boldsymbol{x}_0 + h(A)\boldsymbol{r}_0,$$

where $h \in \Pi_{m-1}$ is the polynomial interpolating $f(z) = z^{-1}$ at the eigenvalues of $\widetilde{T}_m$, and $h(\widetilde{T}_m) = \widetilde{T}_m^{-1}$. The eigenvalues of $\widetilde{T}_m$ are termed the *harmonic Ritz values* of $A$ [24]. Of course, $\widetilde{\boldsymbol{x}}_m \in \boldsymbol{x}_0 + \mathcal{K}_m(A, \boldsymbol{r}_0)$ as well, and as was observed in [9, 15, 24], $\widetilde{\boldsymbol{x}}_m$ is in fact the GMRES (or, in the HPD case, MINRES) approximation to $A^{-1}\boldsymbol{b}$.

The following lemma also shows that there are further rank-one modifications for which (3) holds.

LEMMA 1.3 (see [7, Lemma 3]). *Let $\boldsymbol{u} \in \mathbb{C}^m$. Denote $\widehat{T}_m := T_m + \boldsymbol{u}\widehat{\boldsymbol{e}}_m^H$. Then for any $q \in \Pi_{m-1}$,*

$$V_m q\big(\widehat{T}_m\big)V_m^H\boldsymbol{r}_0 = q(A)\boldsymbol{r}_0. \tag{4}$$

It is worth mentioning that the only such modifications of $T_m$ for which (4) can be preserved must be rank-one with nonzero entries only in the last column, as stated in the following new result.

LEMMA 1.4. *Let $M \in \mathbb{C}^{m\times m}, m \le \mathrm{gr}_A(\boldsymbol{r}_0)$, and denote $\widehat{T}_m := T_m + M$. If (4) holds for all $q \in \Pi_{m-1}$, then there exists $\boldsymbol{u} \in \mathbb{C}^m$ such that $M = \boldsymbol{u}\widehat{\boldsymbol{e}}_m^H$.*

*Proof.* Equation (4) holding for all $q \in \Pi_{m-1}$ and Lemma 1.1 imply

$$V_m\widehat{T}_m^jV_m^H\boldsymbol{r}_0 = V_mT_m^jV_m^H\boldsymbol{r}_0, \;\; j \in \{0, \dots, m-1\}.$$

Multiplying from the left by $V_m^H$ and noting that $V_m^H\boldsymbol{r}_0 = \|\boldsymbol{r}_0\|_2\widehat{\boldsymbol{e}}_1$, we have that

$$\widehat{T}_m^j\widehat{\boldsymbol{e}}_1 = T_m^j\widehat{\boldsymbol{e}}_1, \;\; j \in \{0, \dots, m-1\}. \tag{5}$$

From this we obtain that $\widehat{T}_m^j\widehat{\boldsymbol{e}}_1 = \widehat{T}_m\widehat{T}_m^{j-1}\widehat{\boldsymbol{e}}_1 = \widehat{T}_mT_m^{j-1}\widehat{\boldsymbol{e}}_1$. Thus, again using (5), it follows that

$$\boldsymbol{0} = (\widehat{T}_m - T_m)T_m^{j-1}\widehat{\boldsymbol{e}}_1 = MT_m^{j-1}\widehat{\boldsymbol{e}}_1, \;\; j \in \{1, \dots, m-1\}. \tag{6}$$

The relation (6) further implies

$$MR = 0 \text{ with } R = [\widehat{\boldsymbol{e}}_1 \mid T_m\widehat{\boldsymbol{e}}_1 \mid \cdots \mid T_m^{m-2}\widehat{\boldsymbol{e}}_1] \in \mathbb{C}^{m\times(m-1)}. \tag{7}$$

Since $T_m^j$ has an entirely nonzero $j$th subdiagonal, with all further subdiagonals being zero, the matrix $R$ is upper triangular with all diagonal elements nonzero. From (7) we thus conclude that only the last ($m$th) column of $M$ is nonzero. ∎

**2. The Radau–Lanczos method for linear systems.** In section 1, we saw that the Lanczos relation for an HPD matrix is related to the CG polynomials, as well as an $m$-point Gauss quadrature rule with respect to the measure $\mathrm{d}\alpha$ and with nodes at the eigenvalues of $T_m$. In this section, we show how a particular $(m+1)$-point Gauss–Radau quadrature rule for a modified measure is related to a rank-one update of the tridiagonal matrix $T_{m+1}$. This modification can, in principle, be used to devise a new iterative method for solving linear systems, as an alternative to CG. For this purpose one would have to work out a stable implementation based on short recurrences—a path which we do not follow in this paper. Rather, the theoretical results derived in this section are needed as building blocks for the more general matrix function case considered in section 3.

In an $m$-point Gauss quadrature rule, the quadrature nodes are determined so that the rule is exact for polynomials up to degree $2m-1$. An $(m+1)$-point Gauss–Radau quadrature rule is a modification of a Gauss rule, in which one quadrature node is fixed and exactness for polynomials of degree up to $2m$ is obtained. We fix $\theta_0 > \lambda_{\max}$, and consider the $(m+1)$-point Gauss–Radau rule on the interval $[\lambda_{\min}, \lambda_{\max}]$ for a new measure $\mathrm{d}\alpha_{\mathrm{R}}$ defined as

$$\mathrm{d}\alpha_{\mathrm{R}}(t) := (\theta_0 - t)\,\mathrm{d}\alpha(t). \tag{8}$$

As is explained in the work of Golub [13] and Golub and Meurant [14], there exists a matrix $T_{m+1}^{\mathrm{R}}$ related to $T_m$ whose eigenvalues are the nodes of this rule. Writing

$$T_m = \begin{bmatrix} \omega_1 & \gamma_1 & & & \\ \gamma_1 & \omega_2 & \gamma_2 & & \\ & \ddots & \ddots & \ddots & \\ & & \gamma_{m-2} & \omega_{m-1} & \gamma_{m-1} \\ & & & \gamma_{m-1} & \omega_m \end{bmatrix}, \tag{9}$$

we solve for $\boldsymbol{d} \in \mathbb{C}^m$ satisfying $(T_m - \theta_0 I)\boldsymbol{d} = \gamma_m^2 \widehat{\boldsymbol{e}}_m$ and define

$$T_{m+1}^{\mathrm{R}} := \begin{bmatrix} T_m & \gamma_m \widehat{\boldsymbol{e}}_m \\ \gamma_m \widehat{\boldsymbol{e}}_m^H & d_m + \theta_0 \end{bmatrix}, \tag{10}$$

where $d_m$ is the $m$th component of $\boldsymbol{d}$. Note that $T_{m+1}^{\mathrm{R}}$ is a rank-one modification of $T_{m+1}$, namely, $T_{m+1}^{\mathrm{R}} = T_{m+1} + (d_m - \omega_{m+1})\widehat{\boldsymbol{e}}_{m+1}\widehat{\boldsymbol{e}}_{m+1}^H$, which satisfies the hypotheses of Lemma 1.3. The eigenvalues of $T_{m+1}^{\mathrm{R}}$ are the nodes of the $(m+1)$-point Gauss–Radau rule, with one eigenvalue being equal to $\theta_0$. We denote the eigenvalues of $T_{m+1}^{\mathrm{R}}$ different from $\theta_0$ by $\theta_{m,i}^{\mathrm{R}}$, $i = 1, \ldots, m$. Note that for each $m$, there is a different set of eigenvalues $\theta_{m,i}^{\mathrm{R}}$ even though $\theta_0$ remains the same.

As with CG, there is a connection to a particular set of orthogonal polynomials, given the appropriate inner product in $\Pi_m$. According to Gautschi [12], this inner product is

$$(p,q)_{\mathrm{R}} := \sum_{i=1}^{n} |\beta_i|^2 (\theta_0 - \lambda_i)\bar{p}(\lambda_i) q(\lambda_i) = \int_{\lambda_{\min}}^{\lambda_{\max}} \bar{p}(z) q(z)\,\mathrm{d}\alpha_{\mathrm{R}}(z), \tag{11}$$

which we refer to as the *Radau inner product*, with $\mathrm{d}\alpha_{\mathrm{R}}$ as the *Radau measure* defined in (8). We let $p_m^{\mathrm{R}}$ denote the polynomials orthogonal with respect to this inner product, whose roots are $\theta_{m,i}^{\mathrm{R}}$, $i = 1, \ldots, m$. Note that $\theta_0$ is not a root of $p_m^{\mathrm{R}}$ for any $m$.

We finally define the $(m+1)$st Radau–Lanczos approximation to $A^{-1}\boldsymbol{b}$ as

$$\boldsymbol{x}_{m+1}^{\mathrm{R}} := \boldsymbol{x}_0 + V_{m+1}\big(T_{m+1}^{\mathrm{R}}\big)^{-1} V_{m+1}^H \boldsymbol{r}_0.$$

Computing $T_{m+1}^{\mathrm{R}}$ costs little additional effort, since $m$ is typically very small in comparison to $n$, the size of $A$. Therefore, one iteration of the Radau–Lanczos method takes roughly the same amount of computational effort as one iteration of the standard Lanczos method.

As in section 1, there is a relation between interpolating polynomials for $z^{-1}$ and orthogonal polynomials, now with respect to the Radau inner product, i.e., the polynomials $p_m^{\mathrm{R}}$. Let $q_m^{\mathrm{R}}$ denote the polynomial of degree $m$ which interpolates $f(z) = z^{-1}$ at the eigenvalues of $T_{m+1}^{\mathrm{R}}$. By Lemma 1.3,

$$\boldsymbol{x}_{m+1}^{\mathrm{R}} = \boldsymbol{x}_0 + V_{m+1} q_m^{\mathrm{R}}\big(T_{m+1}^{\mathrm{R}}\big) V_{m+1}^H \boldsymbol{r}_0 = \boldsymbol{x}_0 + q_m^{\mathrm{R}}(A)\boldsymbol{r}_0.$$

Then

$$\boldsymbol{e}_{m+1}^{\mathrm{R}} = \boldsymbol{e}_0 - q_m^{\mathrm{R}}(A)\boldsymbol{r}_0 = \boldsymbol{e}_0 - A q_m^{\mathrm{R}}(A)\boldsymbol{e}_0 = \pi_{m+1}^{\mathrm{R}}(A)\boldsymbol{e}_0,$$

where $\pi_{m+1}^{\mathrm{R}}(z) := 1 - z q_m^{\mathrm{R}}(z)$ and $\pi_{m+1}^{\mathrm{R}} \in \Pi_{m+1}$. Consequently, $\boldsymbol{r}_{m+1}^{\mathrm{R}} = \pi_{m+1}^{\mathrm{R}}(A)\boldsymbol{r}_0$. Note that

$$\pi_{m+1}^{\mathrm{R}}(z) = \left(1 - \frac{z}{\theta_0}\right)\widetilde{p}_m^{\mathrm{R}}(z), \quad \text{where} \quad \widetilde{p}_m^{\mathrm{R}}(z) = \frac{1}{p_m^{\mathrm{R}}(0)} p_m^{\mathrm{R}}(z), \tag{12}$$

since the roots of $\pi_{m+1}^{\mathrm{R}}$ are the eigenvalues of $T_{m+1}^{\mathrm{R}}$ and $\pi_{m+1}^{\mathrm{R}}(0) = 1$.

**2.1. Variational characterization.** We further derive a variational characterization of the Radau–Lanczos method, via a useful orthogonality property.

LEMMA 2.1. *For any* $s \in \Pi_{m-1}$, $\langle \boldsymbol{e}_0 - q_m^{\mathrm{R}}(A)\boldsymbol{r}_0, s(A)\boldsymbol{r}_0 \rangle_A = 0$.

*Proof.* The proof follows from the definition (11) and the polynomial equivalence (12):

$$\begin{aligned} 0 = ({\theta_0}^{-1}\widetilde{p}_m^{\mathrm{R}}, s)_{\mathrm{R}} \;&=\; \sum_{i=1}^{n} |\beta_i|^2 \, (\theta_0 - \lambda_i){\theta_0}^{-1}\widetilde{\overline{p}}_m^{\mathrm{R}}(\lambda_i) s(\lambda_i) \\ &= \langle (\theta_0 I - A){\theta_0}^{-1}\widetilde{p}_m^{\mathrm{R}}(A)\boldsymbol{r}_0, s(A)\boldsymbol{r}_0 \rangle_2 \;=\; \langle \pi_{m+1}^{\mathrm{R}}(A)\boldsymbol{r}_0, s(A)\boldsymbol{r}_0 \rangle_2 \\ &= \langle A(\boldsymbol{e}_0 - q_m^{\mathrm{R}}(A)\boldsymbol{r}_0), s(A)\boldsymbol{r}_0 \rangle_2 \;=\; \langle \boldsymbol{e}_0 - q_m^{\mathrm{R}}(A)\boldsymbol{r}_0, s(A)\boldsymbol{r}_0 \rangle_A. \end{aligned}$$ ∎

By definition, $q_m^{\mathrm{R}}$ interpolates $z^{-1}$ at the eigenvalues of $T_{m+1}^{\mathrm{R}}$. In particular, for every $m$, $q_m^{\mathrm{R}}$ interpolates $z^{-1}$ at $\theta_0$; i.e., for all $m$ there exists $s_{m-1}^{\mathrm{R}} \in \Pi_{m-1}$ such that

$$q_m^{\mathrm{R}}(z) = (\theta_0 - z)s_{m-1}^{\mathrm{R}}(z) + \frac{1}{\theta_0}. \tag{13}$$

Thus, $q_m^{\mathrm{R}}$, a polynomial of degree $m$, is completely determined by the polynomial $s_{m-1}^{\mathrm{R}}$ of degree $m-1$. It is precisely this fact that leads to the following variational characterization of the Radau–Lanczos method.

THEOREM 2.2. *The error* $\boldsymbol{e}_{m+1}^{\mathrm{R}} = \boldsymbol{x}_* - \boldsymbol{x}_{m+1}^{\mathrm{R}}$ *of the approximation* $\boldsymbol{x}_{m+1}^{\mathrm{R}}$ *satisfies*

$$\left\|\boldsymbol{e}_{m+1}^{\mathrm{R}}\right\|_{A(\theta_0 I - A)^{-1}} = \min_{\substack{p \in \Pi_{m+1} \\ p(0)=1, p(\theta_0)=0}} \|p(A)\boldsymbol{e}_0\|_{A(\theta_0 I - A)^{-1}}.$$

*Proof.* By Lemma 2.1 and (13), the error $\boldsymbol{e}_{m+1}^{\mathrm{R}} = \boldsymbol{e}_0 - q_m^{\mathrm{R}}(A)\boldsymbol{r}_0$ satisfies, for all $s \in \Pi_{m-1}$,

$$\begin{aligned}
0 &= \langle \boldsymbol{e}_0 - q_m^{\mathrm{R}}(A)\boldsymbol{r}_0, s(A)\boldsymbol{r}_0 \rangle_A \\
&= \langle \boldsymbol{e}_0 - \frac{1}{\theta_0}\boldsymbol{r}_0 - (\theta_0 I - A)s_{m-1}^{\mathrm{R}}(A)\boldsymbol{r}_0, s(A)\boldsymbol{r}_0 \rangle_A \\
&= \langle \boldsymbol{e}_0 - \frac{1}{\theta_0}\boldsymbol{r}_0 - (\theta_0 I - A)s_{m-1}^{\mathrm{R}}(A)\boldsymbol{r}_0, (\theta_0 I - A)s(A)\boldsymbol{r}_0 \rangle_{A(\theta_0 I - A)^{-1}}.
\end{aligned}$$

Since $(\theta_0 I - A)s_{m-1}^{\mathrm{R}}(A)\boldsymbol{r}_0 \in (\theta_0 I - A)\mathcal{K}_m(A, \boldsymbol{r}_0)$, and since $(\theta_0 I - A)s(A)\boldsymbol{r}_0$ with $s \in \Pi_{m-1}$ describes all the elements of $(\theta_0 I - A)\mathcal{K}_m(A, \boldsymbol{r}_0)$, this gives the following variational characterization of the error:

$$\left\|\boldsymbol{e}_{m+1}^{\mathrm{R}}\right\|_{A(\theta_0 I - A)^{-1}} = \min_{\boldsymbol{y} \in (\theta_0 I - A)\mathcal{K}_m(A, \boldsymbol{r}_0)} \left\| \boldsymbol{e}_0 - \frac{1}{\theta_0}\boldsymbol{r}_0 - \boldsymbol{y} \right\|_{A(\theta_0 I - A)^{-1}}.$$

Since $\boldsymbol{y} \in (\theta_0 I - A)\mathcal{K}_m(A, \boldsymbol{r}_0)$ if and only if $\boldsymbol{y} = (\theta_0 I - A)s_{m-1}(A)\boldsymbol{r}_0$ for some polynomial $s_{m-1} \in \Pi_{m-1}$, we have

$$\boldsymbol{e}_0 - \frac{1}{\theta_0}\boldsymbol{r}_0 - \boldsymbol{y} = \boldsymbol{e}_0 - \frac{1}{\theta_0}A\boldsymbol{e}_0 - (\theta_0 I - A)s_{m-1}(A)A\boldsymbol{e}_0 = \pi_m(A)\boldsymbol{e}_0,$$

where $\pi_m(z) = (1 - \frac{z}{\theta_0})(1 - \theta_0 \cdot z s_{m-1}(z))$. The assertion of the theorem now follows from observing that

$$\{(1 - \tfrac{z}{\theta_0})(1 - \theta_0 z s(z)) : s \in \Pi_{m-1}\} = \{p(z) : p \in \Pi_{m+1}, p(0) = 1, p(\theta_0) = 0\}. \qquad \square$$

**2.2. Finite termination property and error bounds.** It is well known for CG that, in exact arithmetic, the true solution of (1) is obtained in precisely $\widehat{m} := \mathrm{gr}_A(\boldsymbol{r}_0)$ steps. Since the Radau–Lanczos method also relies on the Lanczos relation, it cannot run beyond iteration $\widehat{m}+1$. From the discussion of the Lanczos relation (2) and with the notation from (9) we see that $\gamma_{\widehat{m}} = 0$ and that $T_{\widehat{m}+1}^{\mathrm{R}}$ are thus given as

$$T_{\widehat{m}+1}^{\mathrm{R}} = \begin{bmatrix} T_{\widehat{m}} & \mathbf{0} \\ \mathbf{0} & \theta_0 \end{bmatrix}.$$

If we formally define $V_{\widehat{m}+1} = [V_{\widehat{m}} \mid \mathbf{0}]$ we then have

$$\boldsymbol{x}_0 + V_{\widehat{m}+1}\left(T_{\widehat{m}+1}^{\mathrm{R}}\right)^{-1}V_{\widehat{m}+1}^H \boldsymbol{r}_0 \;=\; \boldsymbol{x}_0 + V_{\widehat{m}}\left(T_{\widehat{m}}\right)^{-1}V_{\widehat{m}}^H \boldsymbol{r}_0 \;=\; A^{-1}\boldsymbol{b},$$

showing that iteration $\widehat{m}+1$ of the Radau–Lanczos method retrieves the exact solution (provided we set the $(\widehat{m}+1)$st Lanczos vector to $\mathbf{0}$).

We can further give an upper bound for the norm of the $m$th Radau–Lanczos error, similar to the classical bounds for the energy norm of the CG error. Define the following quantities:

$$\kappa := \frac{\lambda_{\max}}{\lambda_{\min}}, \quad c := \frac{\sqrt{\kappa} - 1}{\sqrt{\kappa} + 1}, \quad \text{and} \quad \xi_m := \frac{1}{\cosh(m \ln c)}. \tag{14}$$

If $\kappa = 1$, then we set $\xi_m = 0$.

THEOREM 2.3. *The norm of the error of the Radau–Lanczos approximation* $\boldsymbol{x}_{m+1}^{\mathrm{R}}$ *can be bounded as*

$$\begin{aligned}\left\|\boldsymbol{e}_{m+1}^{\mathrm{R}}\right\|_{A(\theta_0 I-A)^{-1}} &\le \left(1-\frac{\lambda_{\min}}{\theta_0}\right)\xi_m \left\|\boldsymbol{e}_0\right\|_{A(\theta_0 I-A)^{-1}}\\ &\le 2\left(1-\frac{\lambda_{\min}}{\theta_0}\right)c^m \left\|\boldsymbol{e}_0\right\|_{A(\theta_0 I-A)^{-1}}.\end{aligned}$$

*Proof.* For ease of notation, let $\widehat{A} := A(\theta_0 I - A)^{-1}$. Since the matrix $\widehat{A}^{\frac{1}{2}}$ commutes with $(\theta_0 I - A)p(A)$ for any polynomial $p$, we have

$$\begin{aligned}\|(\theta_0 I - A)p(A)\|_{\widehat{A}} &= \left\|\widehat{A}^{\frac{1}{2}}(\theta_0 I - A)p(A)\widehat{A}^{-\frac{1}{2}}\right\|_2\\ &= \|(\theta_0 I - A)p(A)\|_2 .\end{aligned}$$

Then by applying Theorem 2.2, we obtain that

$$\begin{aligned}\left\|\boldsymbol{e}_{m+1}^{\mathrm{R}}\right\|_{\widehat{A}} &= \min_{\substack{p\in\Pi_{m+1}\\ p(0)=1,p(\theta_0)=0}} \|p(A)\boldsymbol{e}_0\|_{\widehat{A}}\\
&= \min_{\substack{p\in\Pi_m\\ p(0)=1}} \left\|(I-\tfrac{1}{\theta_0}A)p(A)\boldsymbol{e}_0\right\|_{\widehat{A}}\\
&\le \min_{\substack{p\in\Pi_m\\ p(0)=1}} \left\|(I-\tfrac{1}{\theta_0}A)p(A)\right\|_{\widehat{A}} \|\boldsymbol{e}_0\|_{\widehat{A}}\\
&= \min_{\substack{p\in\Pi_m\\ p(0)=1}} \left\|(I-\tfrac{1}{\theta_0}A)p(A)\right\|_2 \|\boldsymbol{e}_0\|_{\widehat{A}}\\
&\le \min_{\substack{p\in\Pi_m\\ p(0)=1}} \max_{\lambda\in[\lambda_{\min},\lambda_{\max}]} (1-\tfrac{\lambda}{\theta_0})\,|p(\lambda)|\,\|\boldsymbol{e}_0\|_{\widehat{A}}\end{aligned}$$

$$\le \left(1-\frac{\lambda_{\min}}{\theta_0}\right)\cdot \min_{\substack{p\in\Pi_m\\ p(0)=1}} \max_{\lambda\in[\lambda_{\min},\lambda_{\max}]} |p(\lambda)|\,\|\boldsymbol{e}_0\|_{\widehat{A}} . \tag{15}$$

An upper bound for (15) is obtained as $\max_{\lambda\in[\lambda_{\min},\lambda_{\max}]}|p(\lambda)|$ with $p$ the scaled Chebyshev polynomial for which one knows (see, e.g., [26, section 6.11]) the following:

$$\max_{\lambda\in[\lambda_{\min},\lambda_{\max}]} |p(\lambda)| \le \xi_m \le 2c^m. \qquad \square$$

**3. The Radau–Lanczos method for Stieltjes functions of matrices.** From this section onward, we will turn our attention to the case of general Stieltjes matrix functions instead of the special case of linear systems. We will, however, use the results of section 2 as a foundation for our theory, following a similar path as in [9], where the relation between matrix functions and shifted linear systems is exploited.

Let $f$ be a (Cauchy–)Stieltjes function (sometimes also called a Markov-type function). That is, $f$ can be expressed as a Riemann–Stieltjes integral of the form

$$f(z) = \int_0^\infty \frac{1}{t+z}\ \mathrm{d}\mu(t), \tag{16}$$

where $\mu$ is monotonically increasing and nonnegative on $[0,\infty)$ with the property $\int_0^\infty \frac{1}{t+1}\ \mathrm{d}\mu(t) < \infty$. Define the Radau–Lanczos approximation to $f(A)\boldsymbol{b}$ as

$$\boldsymbol{f}_{m+1}^{\mathrm{R}} := V_{m+1} f(T_{m+1}^{\mathrm{R}}) V_{m+1}^H \boldsymbol{b}.$$

Note that $f(T^{\mathrm{R}}_{m+1}) = q_*(T^{\mathrm{R}}_{m+1})$, where $q_* \in \Pi_m$ is the polynomial which interpolates $f$ at the eigenvalues of $T^{\mathrm{R}}_{m+1}$. This equality can be proven in the same manner as the corresponding result for the standard Lanczos method; see, e.g., [25]. By Lemma 1.3, $\boldsymbol{f}^{\mathrm{R}}_{m+1} = q_*(A)\boldsymbol{b} \in (\theta_0 I - A)\mathcal{K}_m(A, \boldsymbol{b})$.

By an argument analogous to that at the beginning of section 2.2, one sees that in exact arithmetic the Radau–Lanczos method for $f(A)\boldsymbol{b}$ will terminate with $\boldsymbol{f}^{\mathrm{R}}_{m+1} = f(A)\boldsymbol{b}$ after exactly $m+1 = \mathrm{gr}_A(\boldsymbol{b}) + 1$ steps. To derive upper bounds for the norm of the error of $\boldsymbol{f}^{\mathrm{R}}_{m+1}$, which will be especially useful for proving convergence of the restarted Radau–Lanczos method later on, we take advantage of the integral form (16) of $f$ in the expressions of $f(A)\boldsymbol{b}$ and $\boldsymbol{f}^{\mathrm{R}}_{m+1}$:

(17)
$$f(A)\boldsymbol{b} = \int_0^\infty (A+tI)^{-1}\boldsymbol{b}\ \mathrm{d}\mu(t) \quad \text{and} \quad \boldsymbol{f}^{\mathrm{R}}_{m+1} = \int_0^\infty V_{m+1}(T^{\mathrm{R}}_{m+1} + tI)^{-1} V_{m+1}^H \boldsymbol{b}\ \mathrm{d}\mu(t).$$

We therefore need shifted versions of the results in section 2.

LEMMA 3.1. *Let $\widehat{T}_m = T_m + \boldsymbol{u}\widehat{\boldsymbol{e}}_m^H$ and $\boldsymbol{r}_0$ be as in Lemma 1.3. Then for all $t \in \mathbb{C}$ and for all $q \in \Pi_{m-1}$,*

$$V_m q(\widehat{T}_m + tI) V_m^H \boldsymbol{r}_0 = q(A+tI)\boldsymbol{r}_0.$$

*Proof.* It is easily verified that the Lanczos relation (2) is shift invariant: $AV_m = V_m T_m + t_{m+1,m}\boldsymbol{v}_{m+1}\widehat{\boldsymbol{e}}_m^H$ implies $(A+tI)V_m = V_m(T_m + tI) + t_{m+1,m}\boldsymbol{v}_{m+1}\widehat{\boldsymbol{e}}_m^H$. Therefore, the columns of $V_m$ are also a basis of $\mathcal{K}_m(A+tI, \boldsymbol{r}_0)$. Applying Lemma 1.3 to $A+tI$ and $\widehat{T}_m + tI$ gives the desired result. ∎

We also define the following shifted quantities for $t \geq 0$:

$$\begin{aligned}
\boldsymbol{x}_*(t) &:= (A+tI)^{-1}\boldsymbol{b},\\
\boldsymbol{x}^{\mathrm{R}}_{m+1}(t) &:= V_{m+1}(T^{\mathrm{R}}_{m+1} + tI)^{-1}V^H_{m+1}\boldsymbol{b},\\
\boldsymbol{e}^{\mathrm{R}}_{m+1}(t) &:= \boldsymbol{x}_*(t) - \boldsymbol{x}^{\mathrm{R}}_{m+1}(t),\\
\boldsymbol{r}^{\mathrm{R}}_{m+1}(t) &:= (A+tI)\boldsymbol{e}^{\mathrm{R}}_{m+1}(t).
\end{aligned} \tag{18}$$

Note that $\boldsymbol{x}^{\mathrm{R}}_{m+1}(t)$ is *not* the $(m+1)$st Radau–Lanczos approximation to $\boldsymbol{x}_*(t)$, although it is *an* approximation to $\boldsymbol{x}_*(t)$. The important property is that the residuals of the iterates $\boldsymbol{x}^{\mathrm{R}}_{m+1}(t)$ belonging to different shifts $t$ are collinear with $\boldsymbol{r}^{\mathrm{R}}_{m+1}(0)$, as stated in the following lemma. We need the case $\boldsymbol{x}^{\mathrm{R}}_0(t) = \boldsymbol{0}$, i.e., $\boldsymbol{r}^{\mathrm{R}}_0(t) = \boldsymbol{b}$ for all $t$, for the convergence result given in Theorem 3.3 below, whereas the more general case is needed later for the analysis of restarts, Theorem 3.6.

LEMMA 3.2. *Consider the family of shifted linear systems $(A+tI)\boldsymbol{x}(t) = \boldsymbol{b}(t)$ with $t \in [0,\infty)$. Assume that we are given initial approximations $\boldsymbol{x}_0(t)$ such that the initial shifted residuals $\boldsymbol{r}^{\mathrm{R}}_0(t)$ are all collinear with $\boldsymbol{r}^{\mathrm{R}}_0(0)$, i.e., $\boldsymbol{r}^{\mathrm{R}}_0(t) = \rho_0(t)\boldsymbol{r}^{\mathrm{R}}_0(0)$ for some $\rho_0(t) \in \mathbb{C}$. Then*

(i) *the residuals $\boldsymbol{r}^{\mathrm{R}}_{m+1}(t)$ for the shifted systems are collinear with $\boldsymbol{r}^{\mathrm{R}}_{m+1}(0)$,*

$$\boldsymbol{r}^{\mathrm{R}}_{m+1}(t) = \rho_{m+1}(t)\boldsymbol{r}^{\mathrm{R}}_{m+1}(0), \quad \textit{where } \rho_{m+1}(t) := \frac{\rho_0(t)}{\pi^{\mathrm{R}}_{m+1}(-t)},$$

*and $\pi^{\mathrm{R}}_{m+1}$ is the polynomial for which $\boldsymbol{r}^{\mathrm{R}}_{m+1} = \pi^{\mathrm{R}}_{m+1}(A)\boldsymbol{r}^{\mathrm{R}}_0(0)$ from (12); and*

(ii) $|\rho_{m+1}(t)| \leq |\rho_0(t)|$.

*Proof.* To show (i) we first apply Lemma 3.1 and relations from section 2 to $A+tI$ and $T^{\mathrm{R}}_{m+1}+tI$ to obtain that

$$\boldsymbol{r}^{\mathrm{R}}_{m+1}(t) = \pi^{\mathrm{R}}_{m+1,t}(A+tI)\boldsymbol{r}^{\mathrm{R}}_{0}(t),$$

where $\pi^{\mathrm{R}}_{m+1,t}(z) = 1 - zq^{\mathrm{R}}_{m,t}(z)$, and $q^{\mathrm{R}}_{m,t} \in \Pi_m$ interpolates $z^{-1}$ at the eigenvalues of $T^{\mathrm{R}}_{m+1}+tI$, which are $\theta_0+t$ and $\theta^{\mathrm{R}}_{m,i}+t$, $i=1,\ldots,m$. Writing $\pi^{\mathrm{R}}_{m+1,t}$ explicitly as

$$\pi^{\mathrm{R}}_{m+1,t}(z) = \frac{(\theta_0+t-z)\prod_{i=1}^{m}(\theta^{\mathrm{R}}_{m,i}+t-z)}{(\theta_0+t)\prod_{i=1}^{m}(\theta^{\mathrm{R}}_{m,i}+t)},$$

one can see that

$$\pi^{\mathrm{R}}_{m+1,t}(z) = \frac{\pi^{\mathrm{R}}_{m+1,0}(z-t)}{\pi^{\mathrm{R}}_{m+1,0}(-t)} = \frac{\pi^{\mathrm{R}}_{m+1}(z-t)}{\pi^{\mathrm{R}}_{m+1}(-t)}.$$

Therefore,

$$\boldsymbol{r}^{\mathrm{R}}_{m+1}(t) = \pi^{\mathrm{R}}_{m+1,t}(A+tI)\boldsymbol{r}^{\mathrm{R}}_{0}(t) = \frac{1}{\pi^{\mathrm{R}}_{m+1}(-t)}\pi^{\mathrm{R}}_{m+1}(A)\boldsymbol{r}^{\mathrm{R}}_{0}(t) = \frac{\rho_0(t)}{\pi^{\mathrm{R}}_{m+1}(-t)}\boldsymbol{r}^{\mathrm{R}}_{m+1}(0),$$

where the last equality holds by the collinearity assumption $\boldsymbol{r}^{\mathrm{R}}_{0}(t) = \rho_0(t)\boldsymbol{r}^{\mathrm{R}}_{0}(0)$ and by the equality $\pi^{\mathrm{R}}_{m+1}(A)\boldsymbol{r}^{\mathrm{R}}_{0}(0) = \boldsymbol{r}^{\mathrm{R}}_{m+1}(0)$.

As for part (ii), since $t \geq 0$ we have

$$|\rho_m(t)| = \frac{|\rho_0(t)|}{|\pi^{\mathrm{R}}_{m+1}(-t)|} = \frac{\theta_0\prod_{i=1}^{m}\theta^{\mathrm{R}}_{m,i}}{(\theta_0+t)\prod_{i=1}^{m}(\theta^{\mathrm{R}}_{m,i}+t)}\rho_0(t) \leq \rho_0(t). \qquad \square$$

At this point, we have all the necessary tools to derive an error bound for the Radau–Lanczos method for Stieltjes functions of HPD matrices. Note that the norm for this error bound is the $A^{-1}(\theta_0 I - A)^{-1}$–norm, which is different from the norm used for the bounds in section 2.

THEOREM 3.3. *The following error bound holds for the Radau–Lanczos method:*

$$\left\|f(A)\boldsymbol{b} - \boldsymbol{f}^{\mathrm{R}}_{m+1}\right\|_{A^{-1}(\theta_0 I - A)^{-1}} \leq C\left(1 - \frac{\lambda_{\min}}{\theta_0}\right)\xi_m \leq 2C\left(1 - \frac{\lambda_{\min}}{\theta_0}\right)c^m,$$

*where $c$ and $\xi_m$ are as in* (14), *and*

$$C \;=\; f(\lambda_{\min})\,\|\boldsymbol{b}\|_{A^{-1}(\theta_0 I - A)^{-1}} \;\leq\; \frac{f(\lambda_{\min})}{\sqrt{\lambda_{\min}(\theta_0 - \lambda_{\max})}}\,\|\boldsymbol{b}\|_2\,.$$

*Proof.* We begin by using (17) to derive an integral expression for the error:

$$f(A)\boldsymbol{b} - \boldsymbol{f}^{\mathrm{R}}_{m+1} = \int_0^\infty \left[\boldsymbol{x}_*(t) - \boldsymbol{x}^{\mathrm{R}}_{m+1}(t)\right]\,\mathrm{d}\mu(t) = \int_0^\infty \boldsymbol{e}^{\mathrm{R}}_{m+1}(t)\,\mathrm{d}\mu(t). \tag{19}$$

Let $\widetilde{A} := A^{-1}(\theta_0 I - A)^{-1}$ and again $\widehat{A} := A(\theta_0 I - A)^{-1}$. Applying Lemma 3.2 to the shifted residuals $\boldsymbol{r}^{\mathrm{R}}_{m+1}(t)$, we obtain the following:

$$\begin{aligned}\left\|f(A)\boldsymbol{b} - \boldsymbol{f}^{\mathrm{R}}_{m+1}\right\|_{\widetilde{A}} &\leq \int_0^\infty \left\|\boldsymbol{e}^{\mathrm{R}}_{m+1}(t)\right\|_{\widetilde{A}} \,\mathrm{d}\mu(t) \\ &= \int_0^\infty \left\|(A+tI)^{-1}\boldsymbol{r}^{\mathrm{R}}_{m+1}(t)\right\|_{\widetilde{A}} \,\mathrm{d}\mu(t) \\ &= \int_0^\infty |\rho_{m+1}(t)| \cdot \left\|(A+tI)^{-1}\boldsymbol{r}^{\mathrm{R}}_{m+1}(0)\right\|_{\widetilde{A}} \,\mathrm{d}\mu(t) \\ &\leq \int_0^\infty |\rho_0(t)| \left\|(A+tI)^{-1}\boldsymbol{r}^{\mathrm{R}}_{m+1}(0)\right\|_{\widetilde{A}} \,\mathrm{d}\mu(t). \qquad (20)\end{aligned}$$

Since $A$, its inverse, and the shifted matrices $A + tI$, $t > 0$, are all HPD, we have the following relation:

$$\begin{aligned}&\left\|(A+tI)^{-1}\boldsymbol{r}^{\mathrm{R}}_{m+1}(0)\right\|^2_{\widetilde{A}} \\ &\quad = \langle (A+tI)^{-1}A\boldsymbol{e}^{\mathrm{R}}_{m+1}(0), A^{-1}(\theta_0 I - A)^{-1}(A+tI)^{-1}A\boldsymbol{e}^{\mathrm{R}}_{m+1}(0)\rangle_2 \\ &\quad \leq \left(\frac{1}{\lambda_{\min} + t}\right)^2 \left\|\boldsymbol{e}^{\mathrm{R}}_{m+1}(0)\right\|^2_{\widehat{A}}. \qquad (21)\end{aligned}$$

Then by applying (21) to the integrand of (20) and by Theorem 2.3, we have

$$\begin{aligned}\left\|f(A)\boldsymbol{b} - \boldsymbol{f}^{\mathrm{R}}_{m+1}\right\|_{\widetilde{A}} &\leq \int_0^\infty \frac{|\rho_0(t)|}{\lambda_{\min}+t} \left\|\boldsymbol{e}^{\mathrm{R}}_{m+1}(0)\right\|_{\widehat{A}} \,\mathrm{d}\mu(t) \\ &\leq \left(1 - \frac{\lambda_{\min}}{\theta_0}\right)\xi_m \left\|\boldsymbol{e}^{\mathrm{R}}_0(0)\right\|_{\widehat{A}} \int_0^\infty \frac{|\rho_0(t)|}{\lambda_{\min}+t} \,\mathrm{d}\mu(t). \qquad (22)\end{aligned}$$

Furthermore, since $\boldsymbol{r}^{\mathrm{R}}_0(t) = \boldsymbol{r}^{\mathrm{R}}_0(0) = \boldsymbol{b}$ for all $t$, we have

$$\begin{aligned}\left\|\boldsymbol{e}^{\mathrm{R}}_0(0)\right\|^2_{\widehat{A}} &= \langle \boldsymbol{e}^{\mathrm{R}}_0(0), \widehat{A}\boldsymbol{e}^{\mathrm{R}}_0(0)\rangle_2 \\ &= \langle \boldsymbol{r}^{\mathrm{R}}_0(0), A^{-1}(\theta_0 I - A)^{-1}\boldsymbol{r}^{\mathrm{R}}_0(0)\rangle_2 \\ &= \|\boldsymbol{b}\|^2_{A^{-1}(\theta_0 I - A)^{-1}} \\ &\leq \frac{1}{\lambda_{\min}(\theta_0 - \lambda_{\max})} \|\boldsymbol{b}\|^2_2. \qquad (23)\end{aligned}$$

Combining (22) and (23), together with the fact that $\rho_0(t) = 1$ for all $t$, we obtain the desired bound. ∎

**3.1. The restarted Radau–Lanczos method.** In many practical situations where one wants to approximate $f(A)\boldsymbol{b}$, the available storage limits the number of Lanczos iterations that can be performed, as one needs to store the entire basis $V_m$ in order to form $\boldsymbol{f}_m$. Therefore, *restarts* are of vital importance in this setting; see, e.g., [1, 5, 9, 10, 21]. The idea is as follows: after a (small) number $m$ of Lanczos steps, one forms a first approximation $\boldsymbol{f}^{(1)}_m$ for $f(A)\boldsymbol{b}$. If this approximation is not accurate enough, one uses $m$ further Lanczos steps (the next *cycle* of the method) to obtain an approximation $\boldsymbol{a}^{(1)}_m$ to the error $f(A)\boldsymbol{b} - \boldsymbol{f}^{(1)}_m$, which is then used as an additive correction to form $\boldsymbol{f}^{(2)}_m = \boldsymbol{f}^{(1)}_m + \boldsymbol{a}^{(1)}_m$. Continuing like this, we obtain the sequences $\boldsymbol{f}^{(k)}_m$ and $\boldsymbol{a}^{(k)}_m$, where $k$ denotes the index of the restart cycle, and $m$ the length of the cycle (i.e., the number of Lanczos steps). We can apply this approach to the Radau–Lanczos method, as long as we can devise a stable and efficient way for computing the error approximations $\boldsymbol{a}^{(k)}_m$. For that, we follow [10], which derives an integral representation of the error and then uses it to compute $\boldsymbol{a}^{(k)}_m$.

The error representation (19) can be rewritten as

$$f(A)\boldsymbol{b} - \boldsymbol{f}_{m+1}^{\mathrm{R}} = \int_0^\infty (A + tI)^{-1} \boldsymbol{r}_{m+1}^{\mathrm{R}}(t)\,\mathrm{d}\mu(t),$$

which, by Lemma 3.2, can be recast into the form

$$f(A)\boldsymbol{b} - \boldsymbol{f}_{m+1}^{\mathrm{R}} = e_{m+1}(A)\boldsymbol{r}_{m+1}^{\mathrm{R}}(0) \text{ with } e_{m+1}(z) := \int_0^\infty \frac{\rho_{m+1}(t)}{t+z}\,\mathrm{d}\mu(t). \tag{24}$$

In (24), the error is represented as the action of a matrix function in $A$ on the vector $\boldsymbol{r}_{m+1}^{\mathrm{R}}(0)$. Therefore, an approximation for the error can be computed with a new cycle of length $m+1$ of the Radau–Lanczos method for $A$ and $\boldsymbol{r}_{m+1}^{\mathrm{R}}(0)$. To do this, one needs to be able to evaluate the error function on the Hessenberg matrix of the next Radau–Lanczos cycle. As $e_{m+1}$ is only known via its integral representation, for which one usually does not have a closed form available, it is necessary to evaluate it via numerical quadrature. This idea was explored thoroughly in [10] in the context of the standard Lanczos/Arnoldi method, where an algorithm based on adaptive quadrature is developed and suitable quadrature rules for different functions $f$ are discussed. An analogous implementation for the Radau–Lanczos method is given in Algorithm 1. Note that this implementation needs the residuals $\boldsymbol{r}_{m+1}^{\mathrm{R},(k-1)}(0)$ to be defined in analogy to (18); see also Remark 3.5 below.

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**Algorithm 1:** Quadrature-based restarted Radau–Lanczos method for $f(A)\boldsymbol{b}$.

**Given:** $A$, $\boldsymbol{b}$, $f$, $m$, `tol`, $\theta_0$
1. Compute the Lanczos decomposition $AV_m^{(1)} = V_m^{(1)}T_m^{(1)} + t_{m+1,m}^{(1)}\boldsymbol{v}_{m+1}^{(1)}\widehat{\boldsymbol{e}}_m^H$ with respect to $A$ and $\boldsymbol{b}$
2. Compute $T_{m+1}^{\mathrm{R},(1)}$ according to (10)
3. Set $\boldsymbol{f}_{m+1}^{\mathrm{R},(1)} := \|\boldsymbol{b}\|_2 V_{m+1}^{(1)} f\left(T_{m+1}^{\mathrm{R},(1)}\right)\widehat{\boldsymbol{e}}_1$
4. **for** $k = 2, 3, \ldots,$ until convergence **do**
5. Compute the Lanczos decomposition $AV_m^{(k)} = V_m^{(k)}T_m^{(k)} + t_{m+1,m}^{(k)}\boldsymbol{v}_{m+1}^{(k)}\widehat{\boldsymbol{e}}_m^H$. with respect to $A$ and $\boldsymbol{r}_{m+1}^{\mathrm{R},(k-1)}(0)$
6. Compute $T_{m+1}^{\mathrm{R},(k)}$ according to (10)
7. Choose quadrature nodes $t_i$ and weights $\omega_i$, $i = 1, \ldots, \ell$
8. Compute $\boldsymbol{h}_{m+1}^{(k)} := \sum_{i=1}^{\ell} \omega_i \rho_{m+1}^{(k-1)}(t_i)\left(T_{m+1}^{\mathrm{R},(k)} + t_i I\right)^{-1}\widehat{\boldsymbol{e}}_1$.
9. Set $\boldsymbol{f}_{m+1}^{\mathrm{R},(k)} := \boldsymbol{f}_{m+1}^{\mathrm{R},(k-1)} + \|\boldsymbol{b}\|_2 V_{m+1}^{(k)}\boldsymbol{h}_{m+1}^{(k)}$

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For evaluating the quadrature rule in step 8 of Algorithm 1, one needs to know the collinearity factors $\rho_{m+1}^{(k)}(t_i)$ at the quadrature nodes $t_i$. In theory, these can be computed via the formula given in Lemma 3.2(i), involving the Radau–Lanczos polynomial $\pi_{m+1}^{\mathrm{R}}$, but this representation can become unstable in the presence of round-off error for larger values of $m$ (i.e., when a polynomial of high degree is involved). Fortunately, one can alternatively calculate the residual norms (and thus the collinearity factors) by solving small $m \times m$ tridiagonal linear systems, similarly to a well-known result for the standard Lanczos/Arnoldi method; see, e.g., [26, Proposition 6.7] or [10, section 3]. For the sake of notational simplicity, we only state the result for the unrestarted case, as the generalization is straightforward.

LEMMA 3.4. *Define the quantities*

$$\phi_{m+1}(t) = \widehat{\boldsymbol{e}}_{m+1}^H (T_{m+1} + tI)(T_{m+1}^{\mathrm{R}} + tI)^{-1}\widehat{\boldsymbol{e}}_1 \tag{25}$$

*and*

$$\psi_{m+1}(t) = t_{m+2,m+1}\widehat{\boldsymbol{e}}_{m+1}^H (T_{m+1}^{\mathrm{R}} + tI)^{-1}\widehat{\boldsymbol{e}}_1. \tag{26}$$

*Then*

$$\|\boldsymbol{r}_{m+1}^{\mathrm{R}}(t)\|_2 = \sqrt{\|\boldsymbol{b}\|_2^2 \phi_{m+1}(t)^2 + \psi_{m+1}(t)^2}.$$

*Proof.* By definition of $\boldsymbol{x}_{m+1}^{\mathrm{R}}(t)$ and $\boldsymbol{r}_{m+1}^{\mathrm{R}}(t)$, we have

$$\boldsymbol{r}_{m+1}^{\mathrm{R}}(t) = \boldsymbol{b} - \|\boldsymbol{b}\|_2 (A + tI) V_{m+1} (T_{m+1}^{\mathrm{R}} + tI)^{-1}\widehat{\boldsymbol{e}}_1. \tag{27}$$

Inserting the shifted Lanczos relation (2) for $m+2$ steps,

$$(A + tI)V_{m+1} = V_{m+1}(T_{m+1} + tI) + t_{m+2,m+1}\boldsymbol{v}_{m+2}\widehat{\boldsymbol{e}}_{m+1}^H,$$

into (27) yields

$$\begin{aligned}\boldsymbol{r}_{m+1}^{\mathrm{R}}(t) = \boldsymbol{b} - \|\boldsymbol{b}\|_2 V_{m+1}(T_{m+1} + tI)(T_{m+1}^{\mathrm{R}} + tI)^{-1}\widehat{\boldsymbol{e}}_1 \\ - t_{m+2,m+1}\boldsymbol{v}_{m+2}\widehat{\boldsymbol{e}}_{m+1}^H (T_{m+1}^{\mathrm{R}} + tI)^{-1}\widehat{\boldsymbol{e}}_1.\end{aligned}$$

Since $T_{m+1}$ and $T_{m+1}^{\mathrm{R}}$ only differ in their $(m+1, m+1)$ entry, we have that

$$(T_{m+1} + tI)(T_{m+1}^{\mathrm{R}} + tI)^{-1}\widehat{\boldsymbol{e}}_1 = [1, 0, \dots, 0, \phi_{m+1}(t)]^T,$$

which gives

$$\boldsymbol{r}_{m+1}^{\mathrm{R}}(t) = \boldsymbol{b} - \|\boldsymbol{b}\|_2 \big(\boldsymbol{v}_1 + \phi_{m+1}(t)\boldsymbol{v}_{m+1}\big) - \psi_{m+1}(t)\boldsymbol{v}_{m+2}. \tag{28}$$

Using the fact that $\boldsymbol{b} = \|\boldsymbol{b}\|_2 \boldsymbol{v}_1$, (28) simplifies to

$$\boldsymbol{r}_{m+1}^{\mathrm{R}}(t) = -\|\boldsymbol{b}\|_2 \phi_{m+1}(t)\boldsymbol{v}_{m+1} - \psi_{m+1}(t)\boldsymbol{v}_{m+2}. \tag{29}$$

By the orthogonality of the Lanczos basis, relation (29) directly implies the assertion of the lemma. ∎

*Remark* 3.5. Before proceeding, we give a few comments regarding Lemma 3.4. The proof of the lemma relies on the fact that a Lanczos decomposition for $m+2$ steps (i.e., one step more than needed for defining $\boldsymbol{x}_{m+1}^{\mathrm{R}}(t)$) exists. However, this is no restriction: if $\boldsymbol{v}_{m+2}$ cannot be generated, it is because the Radau–Lanczos approximation has already reached its final iteration and, thus, in exact arithmetic, has found $f(A)\boldsymbol{b}$. We also note that despite the need for computing the matrix $T_{m+1}$ and the scalar $t_{m+2,m+1}$, computing residual norms via Lemma 3.4 at the end of a restart cycle does *not* require additional matrix-vector products, since one needs to invest one matrix-vector product for computing $\boldsymbol{r}_{m+1}^{\mathrm{R}}(0)$, the starting vector of the next restart cycle, anyway. Instead, one can compute $\boldsymbol{v}_{m+2}$ to find all the quantities necessary for evaluating (25) and (26) and then compute $\boldsymbol{r}_{m+1}^{\mathrm{R}}(0)$ via (29) without additional matrix-vector products. Thus, the main *additional* computational work required for computing the values $\rho_{m+1}^{(k-1)}(t_i)$ in line 8 of Algorithm 1 consists of solving one tridiagonal linear system and performing one tridiagonal matrix vector product (each with a matrix of size $m \times m$) per quadrature node. Consequently, the cost for computing the values at all quadrature nodes is $\mathcal{O}(m\ell)$, which is the same as for the standard quadrature-based restarted Lanczos method from [10]. There it was also observed that small values of $\ell$ (not more than a few hundred, and typically far less) are necessary to reach an accuracy on the order of $10^{-15}$, and the same holds for the Radau–Lanczos method.

While the Radau–Lanczos method without restarts finds $f(A)\boldsymbol{b}$ after $\mathrm{gr}_A(\boldsymbol{b}) + 1$ steps (cf. section 2.2), we cannot expect the restarted variant to have a finite termination property. The question of whether the iterates of the restarted method converge in the limit can be answered positively for Stieltjes functions and HPD matrices for any restart length $m$, as the following variant of Theorem 3.3 shows. It represents the analogue of a similar result for the standard Lanczos method given in [9].

Theorem 3.6. *Let $k$ be the number of restart cycles, and $m+1$ the length of each cycle. Let $\boldsymbol{f}_{m+1}^{\mathrm{R},(k)}$ denote the restarted Radau–Lanczos approximation after $k$ cycles. Then*

$$\left\| f(A)\boldsymbol{b} - \boldsymbol{f}_{m+1}^{\mathrm{R},(k)} \right\|_{A^{-1}(\theta_0 I - A)^{-1}} \leq C \left(1 - \frac{\lambda_{\min}}{\theta_0}\right)^k \xi_m^k, \tag{30}$$

*where $C$ is as in Theorem* 3.3 *and $\xi_m$ is as in* (14).

*Proof.* As with $\boldsymbol{f}_{m+1}^{\mathrm{R},(k)}$, we let the superscript $(k)$ denote all the corresponding restarted quantities. Again let $\widetilde{A} := A^{-1}(\theta_0 I - A)^{-1}$ and $\widehat{A} := A(\theta_0 I - A)^{-1}$. Following the proof of Theorem 3.3, we again note that

$$\left\| f(A)\boldsymbol{b} - \boldsymbol{f}_{m+1}^{\mathrm{R},(k)} \right\|_{\widetilde{A}} \leq \int_0^\infty \left\| (A + tI)^{-1} \boldsymbol{r}_{m+1}^{\mathrm{R},(k)}(t) \right\|_{\widetilde{A}} \; \mathrm{d}\mu(t).$$

Assuming the restarted initial residuals are collinear, i.e.,

$$\boldsymbol{r}_0^{\mathrm{R},(k)}(t) = \rho_0^{\mathrm{R},(k)}(t) \boldsymbol{r}_0^{\mathrm{R},(k)}(0),$$

then by Lemma 3.2(i), we have that $\boldsymbol{r}_{m+1}^{\mathrm{R},(k)}(t) = \rho_{m+1}^{\mathrm{R},(k)}(t) \boldsymbol{r}_{m+1}^{\mathrm{R},(k)}(0)$. Furthermore,

$$\begin{aligned} \left\| (A + tI)^{-1} \boldsymbol{r}_{m+1}^{\mathrm{R},(k)}(0) \right\|_{\widetilde{A}} &\leq \frac{1}{\lambda_{\min} + t} \left\| \boldsymbol{e}_{m+1}^{\mathrm{R},(k)}(0) \right\|_{\widehat{A}} \\ &\leq \frac{1}{\lambda_{\min} + t} \left(1 - \frac{\lambda_{\min}}{\theta_0}\right) \xi_m \left\| \boldsymbol{e}_0^{\mathrm{R},(k)}(0) \right\|_{\widehat{A}}, \end{aligned}$$

where the last inequality holds by Theorem 2.3 for a particular restart cycle $k$. Since $\boldsymbol{e}_0^{\mathrm{R},(k)}(0) = \boldsymbol{e}_{m+1}^{\mathrm{R},(k-1)}(0)$, we can apply Theorem 2.3 and Lemma 3.2(i) inductively to obtain

$$\left\| \boldsymbol{e}_0^{\mathrm{R},(k)}(0) \right\|_{\widehat{A}} \leq \left(1 - \frac{\lambda_{\min}}{\theta_0}\right)^{k-1} \xi_m^{k-1} |\rho_{m+1}^{(1)}(t) \cdots \rho_{m+1}^{(k-1)}(t)| \left\| \boldsymbol{e}_0^{(1)}(0) \right\|_{\widehat{A}}.$$

Further note that $\rho_{m+1}^{(i)} = \rho_0^{(i+1)}$; therefore, by repeated application of Lemma 3.2(ii),

$$|\rho_{m+1}^{(1)}(t) \cdots \rho_{m+1}^{(k-1)}(t)| \leq |\rho_0(t)|^{k-1} = 1,$$

since $\rho_0$ is as in Theorem 3.3. Combining all these pieces, we have that

$$\left\| f(A)\boldsymbol{b} - \boldsymbol{f}_{m+1}^{\mathrm{R},(k)} \right\|_{\widehat{A}} \leq \int_0^\infty \frac{1}{\lambda_{\min} + t} \left(1 - \frac{\lambda_{\min}}{\theta_0}\right)^k \xi_m^k \left\| \boldsymbol{e}_0^{(1)}(0) \right\|_{\widehat{A}} \mathrm{d}\mu(t).$$

Using (23) again, we obtain the desired result. ◻

*Remark* 3.7. Before proceeding, we make three comments concerning the result of Theorem 3.6:

1. The bound (30) is minimal when $\theta_0$ takes its smallest admissible value. We have to assume $\theta_0 > \lambda_{\max}$ to keep the Radau inner product positive definite, since otherwise much of our theory would be invalid. Consequently, one should try to choose $\theta_0$ close to but not equal to $\lambda_{\max}$.
2. As for the standard bound for the error in the CG method and the bounds derived from it for the restarted Lanczos method in [9], one cannot expect the bound (30) to be sharp in general. One reason is that the standard bound does not take into account the distribution of the eigenvalues in the interval $[\lambda_{\min}, \lambda_{\max}]$. Moreover, the constant $C$ is mostly an artifact of the technique of proof, so that the order of magnitude of the error is typically severely overestimated.
3. A comparison of the bound (30) with bounds for the standard restarted Lanczos method is not very enlightening as far as the actual behavior of the method is concerned. Both bounds only differ by the factor $(1 - \lambda_{\min}/\theta_0)$, which is very close to 1 for matrices with large condition number. Despite this fact, the actual performance of the methods can be very different in practice. Understanding this behavior is the topic of the next section.

Remark 3.7 stresses that the main implication of Theorem 3.6 is that using the Radau modification cannot destroy the guaranteed convergence of the restarted Lanczos method. The theorem cannot, however, accurately predict the speed of convergence of the method.

**4. Numerical results I: Polynomial studies.** While the theory developed in section 3 for the restarted Radau–Lanczos method guarantees convergence to $f(A)\boldsymbol{b}$, when $A$ is HPD and $f$ is a Stieltjes function, it does not fully explain the behavior observed in numerical experiments, especially when compared to the standard Lanczos method; cf. also Remark 3.7. It is beyond the scope of this paper to perform a rigorous theoretical analysis of the different phenomena one can observe. Rather, we perform a series of academic numerical experiments in this section, in order to shed some light on different features of the method.

In all experiments in this section, we approximate $A^{-1/2}\boldsymbol{b}$, where $\boldsymbol{b} \in \mathbb{R}^{100}$ is the normalized vector of all ones and $A \in \mathbb{R}^{100\times 100}$ is a diagonal matrix with $\lambda_{\min} = 10^{-2}$ and $\lambda_{\max} = 10^2$, i.e., with condition number $\kappa = 10^4$. The inverse square root is indeed a Stieltjes function of the form (16). More generally, for all $\sigma \in (0, 1)$,

$$z^{-\sigma} = \frac{\sin(\sigma\pi)}{\pi} \int_0^\infty \frac{t^{-\sigma}}{t + z} \, \mathrm{d}t$$

is a Stieltjes function; see, e.g., [16].

We use a restart length of $m = 10$ and aim for an absolute error norm below $10^{-10}$. The fixed node in the Radau–Lanczos method is chosen as $\theta_0 = \lambda_{\max} + \lambda_{\min}$. The distribution of the eigenvalues of $A$ in the spectral interval $[10^{-2}, 10^2]$ is chosen in three different ways:

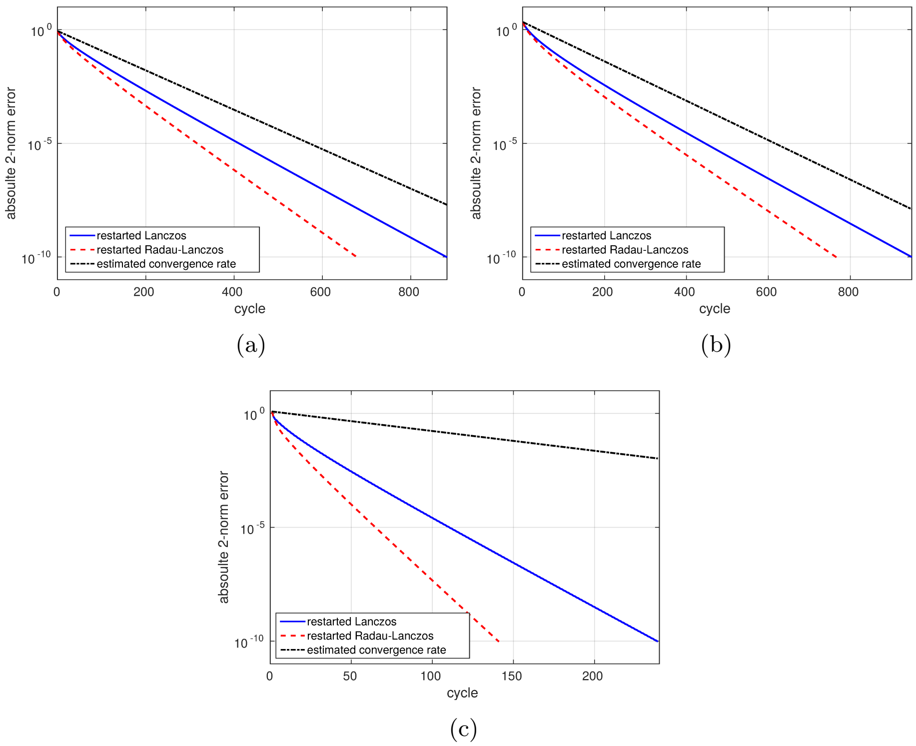


FIG. 1. *Comparison of the convergence behavior of the restarted Lanczos and Radau–Lanczos methods with restart length $m = 10$ for three different diagonal matrices $A$. (See the text for details on the spectra of the matrices.) In addition, the bound for the convergence rate from Theorem* 3.6 *is shown.*

(a) 100 equidistantly spaced eigenvalues in $[10^{-2}, 10^{2}]$;
(b) 100 logarithmically spaced eigenvalues in $[10^{-2}, 10^{2}]$;
(c) 50 equidistantly spaced eigenvalues in $[10^{-2}, 10^{-1}]$ and $[10^{1}, 10^{2}]$ each.

Figure 1 depicts the convergence history of the restarted Lanczos and Radau–Lanczos methods for the three different choices of $A$. The fixed node in the Radau–Lanczos method is chosen as $\lambda_{\max} + \lambda_{\min}$ in all three examples. We observe that the Radau–Lanczos method outperforms the standard Lanczos method in all three cases, although by vastly different margins. Note that this also results in a similar improvement in execution times, since each iteration requires roughly the same amount of computational effort. In order to confirm what we mentioned in Remark 3.7, we also plot the asymptotic convergence factor from the bound from Theorem 3.6. For better readability of the plot, we left out the constant $C$ from (30) as well as the additional constant introduced by transforming the estimate in the $A^{-1}(\theta_0 I - A)^{-1}$-norm into one in the Euclidean norm. In reality, the norm of the error is overestimated by two to three orders of magnitude due to these constants. As the bound (30) only depends on the extremal eigenvalues $\lambda_{\min}$ and $\lambda_{\max}$ of $A$ and the choice of $\theta_0$, it is the same for all three matrices. As expected, the slope of the convergence curve is not resolved very accurately, especially in case $(c)$, where the distribution of the eigenvalues in the interval $[\lambda_{\min}, \lambda_{\max}]$ is such that the Chebyshev polynomials, on which the bounds from Theorem 3.6 are based, are far from being optimal.

A first, intuitive explanation for the improved performance of the Radau–Lanczos method over the standard one is that the largest Ritz value produced by the restarted

Lanczos method with a short cycle length may fail to approximate the largest eigenvalue of $A$ to sufficient accuracy. In this case, the value $|q_{m-1}(\lambda_{\max})|$, where $q_{m-1}$ is the polynomial interpolating $f$ at the Ritz values, may be very large, while $f$ is monotonically decreasing and thus takes its smallest value on $[\lambda_{\min}, \lambda_{\max}]$ at $\lambda_{\max}$. One can therefore expect a large relative error at this point. To confirm this intuition and to better explain the different behavior observed in Figures 1(a)–(c), we compare the interpolating polynomials corresponding to the different methods.

Figure 2 depicts the relative errors of the values of the interpolating polynomials at the eigenvalues $\lambda_{\min} = \lambda_1 \leq \lambda_2 \leq \cdots \leq \lambda_{100} = \lambda_{\max}$ of $A$, i.e., the quantities:

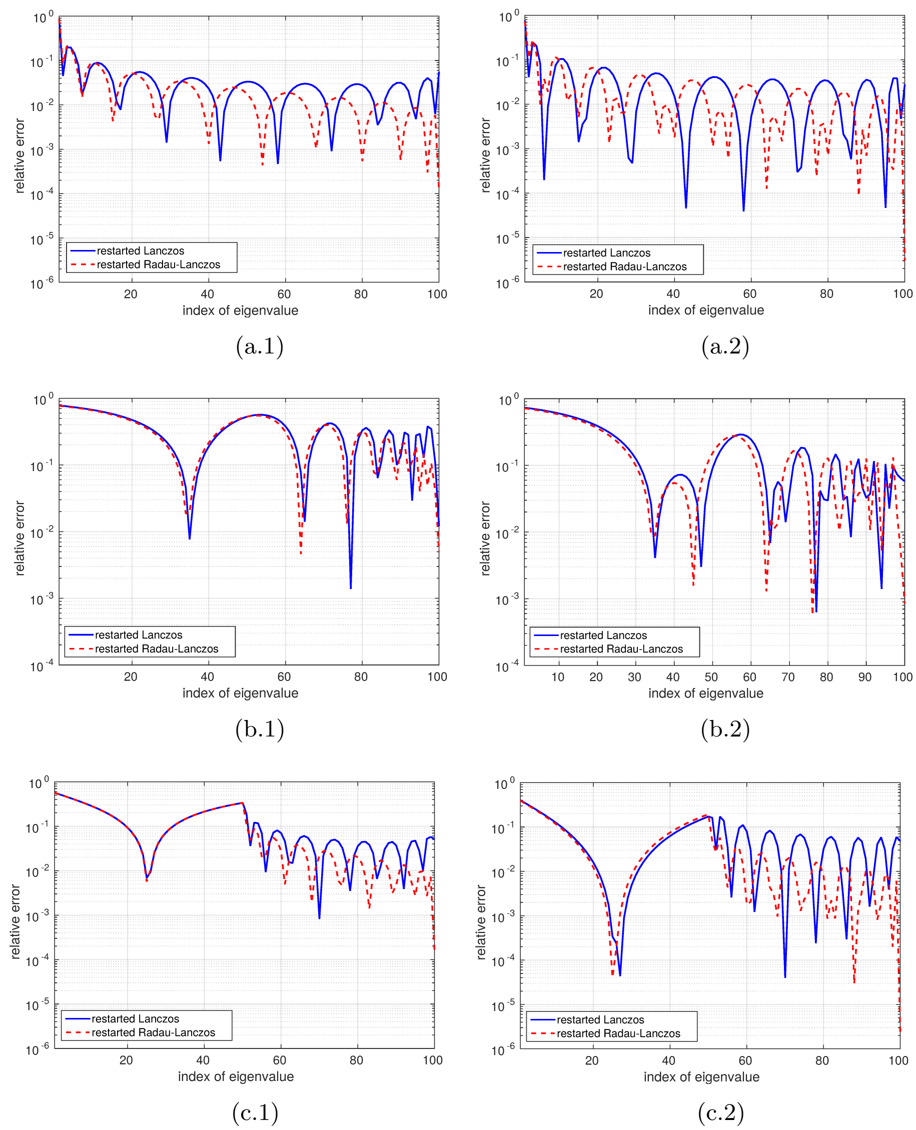


FIG. 2. *Relative errors* $|\lambda_i^{-1/2} - p(\lambda_i)|/\lambda_i^{-1/2}$, $i = 1, \ldots, 100$, *of the interpolating polynomials from the first and second restart cycles, respectively, at the eigenvalues* $\lambda_{\min} = \lambda_1 \leq \lambda_2 \leq \cdots \leq \lambda_{100} = \lambda_{\max}$ *of diagonal matrices with equidistantly spaced eigenvalues* (a.1) *and* (a.2); *logarithmically spaced eigenvalues* (b.1) *and* (b.2); *and a gap in the spectrum* (c.1) *and* (c.2). *See the text for more details on the matrices.*

$$|\lambda_i^{-1/2} - q(\lambda_i)|/\lambda_i^{-1/2}, \quad i = 1, \ldots, 100,$$

where $q$ is either $q_{m-1}$ or $q_m^{\mathrm{R}}$, the interpolating polynomials for each respective method in the first two cycles. As expected, the relative error at the largest eigenvalue $\lambda_{100}$ is much larger for the standard Lanczos method. We note that while we only depict the errors of the interpolating polynomials after the first two of many restart cycles, the observed behavior stays the same for subsequent cycles. This behavior can be explained by the fact that the Ritz values produced in restarted methods asymptotically consist of two sets which are repeated cyclically; see, e.g, [1]. Therefore, when the largest eigenvalue is not approximated to sufficient accuracy in the "first few" restart cycles, one cannot expect this to happen in later cycles. Thus, a high polynomial degree is necessary to reduce the error at $\lambda_{\max}$ sufficiently. The largest Ritz value is typically the one which converges to an eigenvalue the fastest among all Ritz values. Thus, if convergence of the largest Ritz value is unsatisfactory, this will also be the case for all the other Ritz values. We focus on the largest eigenvalue here as this is the one where convergence can be improved by our approach. It would be desirable to also improve the convergence of interior eigenvalues, but this would require different techniques, as $\theta_0 > \lambda_{\max}$ is required, and thus no other "target" eigenvalue may be chosen.

To further understand these phenomena, we also note that the largest Ritz value produced throughout *all* restart cycles of the standard Lanczos method is 99.69 for matrix (a), 99.99 for matrix (b), and 99.50 for matrix (c) (rounded to two decimal digits). Thus, in these examples, we see a direct correspondence between the quality of the approximation to the largest eigenvalue and the improvement of the Radau–Lanczos method over the standard one: the better the approximation quality of the largest Ritz value, the smaller the advantage in using the Radau–Lanczos method.

**5. Numerical results II: Model problems.** We now investigate standard model problems and problems coming from real-world applications, to demonstrate that the Radau–Lanczos method also has benefits in these more practical settings. We again use the same default parameters as in the last section—cycle length $m = 10$, target accuracy $10^{-10}$, and $\theta_0 = \lambda_{\min} + \lambda_{\max}$—unless explicitly stated otherwise.

**5.1. Two-dimensional Laplacian.** The first model problem we consider is the standard finite difference discretization of the two-dimensional Laplace operator with homogeneous Dirichlet boundary conditions on a regular square grid with $N+1$ grid points in each spatial dimension. This results in an $N^2 \times N^2$ matrix of the form

$$A = A_{\mathrm{1D}} \otimes I_N + I_N \otimes A_{\mathrm{1D}}, \text{ where } A_{\mathrm{1D}} = (N+1)^2 \begin{bmatrix} 2 & -1 & & \\ -1 & 2 & \ddots & \\ & \ddots & \ddots & -1 \\ & & -1 & 2 \end{bmatrix} \in \mathbb{C}^{N \times N}.$$

We perform experiments on the functions $f_1(z) = z^{-1/2}$ and $f_2(z) = (e^{-s\sqrt{z}} - 1)/z$, with $N = 40$ and $\boldsymbol{b}$ the (normalized) vector of all ones in both cases. The function $f_2$, which plays an important role in the solution of wave equations (see, e.g., [4]) has an integral representation of the form

$$f_2(z) = -\int_0^\infty \frac{1}{z+t} \frac{\sin(s\sqrt{t})}{\pi t}\, \mathrm{d}t. \tag{31}$$

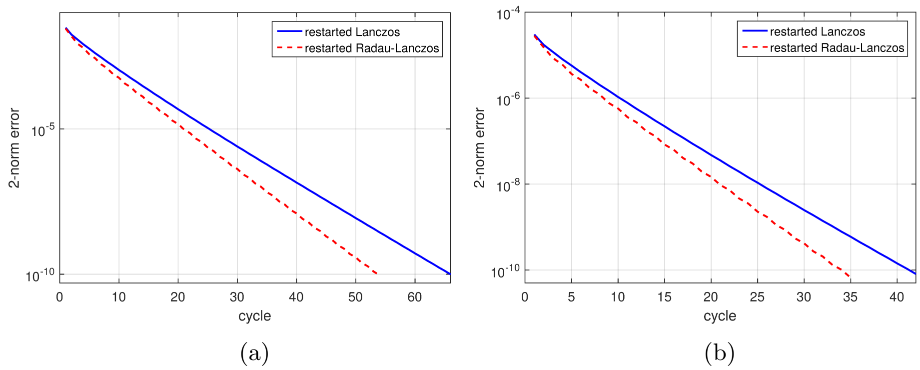


FIG. 3. *Convergence history of the Lanczos and Radau–Lanczos method for approximating* (a) $A^{-1/2}\boldsymbol{b}$ *and* (b) $(e^{-s\sqrt{A}} - I)A^{-1}\boldsymbol{b}$ *for the discretization of the two-dimensional Laplace operator of size* 1,600 × 1,600.

Therefore, $f_2$ is *not* a Stieltjes function, as the function $\mu$ generating $f_2$ is not monotonically increasing. Thus, Theorems 3.3 and 3.6 do not apply, but we can still use a quadrature-based restart approach based on the representation (31); see also [10]. We specify the parameter $s = 0.001$ for $f_2$.

Comparative convergence histories of the Lanczos and Radau–Lanczos methods for these experiments are shown in Figure 3. We observe a similar behavior to the diagonal model problems, with the Radau–Lanczos method requiring about 20% fewer restart cycles than the standard Lanczos method for $f_1$ and about 17% fewer cycles for $f_2$. We note that the maximum eigenvalue of the discretized Laplace operator is explicitly known, so that no additional computational effort must be put into approximating it beforehand.

**5.2. Sampling from Gaussian Markov random fields.** The next model problem is sampling from a Gaussian Markov random field (GMRF), considered in, e.g., [21, 27]. For a set of $n$ points $s_i \in \mathbb{R}^d, i = 1, \ldots, n$, the *precision matrix* $A \in \mathbb{C}^{n\times n}$ (with respect to two parameters $\delta, \phi$) is defined as

$$a_{ij} = \begin{cases} 1 + \phi \sum_{k=1,k\neq i}^{n} \chi_{ik}^{\delta} & \text{if } i = j, \\ -\phi\chi_{ij}^{\delta} & \text{otherwise,} \end{cases}$$

where $\chi^\delta$ is given by

$$\chi_{ij}^{\delta} = \begin{cases} 1 & \text{if } \|s_i - s_j\|_2 < \delta, \\ 0 & \text{otherwise.} \end{cases}$$

This matrix is HPD and strictly diagonally dominant with smallest eigenvalue 1. A GMRF is a collection of random variables $x_i$ corresponding to the points $s_i$. A sample from this field is obtained by computing $A^{-1/2}\boldsymbol{z}$ with $\boldsymbol{z}$ a vector of independently and identically distributed standard normal random variables. We use the precision matrix corresponding to $n = 4{,}000$ pseudorandom points which are uniformly distributed in the unit square (i.e., $d = 2$) with $\phi = 4, \delta = 0.15$. This results in $\lambda_{\max} \approx 1{,}386.4$ and 985,238 nonzeros in $A$. The results of the computations for this model are depicted in Figure 4. We observe a behavior which is very similar to that of the previous model

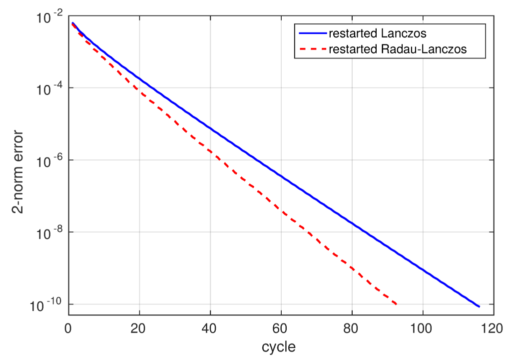


FIG. 4. *Convergence history of the Lanczos and Radau–Lanczos method for approximating* $A^{-1/2}\boldsymbol{z}$ *for a precision matrix of size* $4{,}000 \times 4{,}000$ *of a GMRF and a vector* $\boldsymbol{z}$ *of normal random variables.*

TABLE 1
*Improvement of the restarted Radau–Lanczos method over the standard restarted Lanczos method (in terms of number of restart cycles) for the GMRF model problem, when* $\theta_0 = \beta\lambda_{\max} + \lambda_{\min}$.

| $\beta$ | 1.00 | 1.05 | 1.10 | 1.15 | 1.2 | 1.25 |
|---|---|---|---|---|---|---|
| % reduction of restart cycles | 19.1% | 16.6% | 14.8% | 13.9% | 13.0% | 12.2% |

problem, with the Radau–Lanczos method again showing a decrease of approximately 19% restart cycles.

As the largest eigenvalue of the precision matrix $A$ is not explicitly known in this case, it needs to be approximated (and bounded) beforehand to determine $\theta_0$ to use the Radau–Lanczos method in practice. To illustrate that it is not necessary to approximate the largest eigenvalue very accurately, we repeat the above experiment, but use $\beta\lambda_{\max}$ for different values of $\beta \geq 1$ for defining $\theta_0$. Table 1 shows the improvement of the Radau–Lanczos method over the standard one for different values of $\beta$. While the performance of the Radau–Lanczos method worsens as the approximation to $\lambda_{\max}$ does, it still clearly outperforms the standard method even for $\beta = 1.25$, i.e., when the largest eigenvalue is overestimated by 25%. This shows that the method is robust with respect to this parameter, meaning that rough estimates of $\lambda_{\max}$ are sufficient to see an acceleration in convergence.

**5.3. Rational hybrid Monte Carlo method in lattice QCD.** *Quantum chromodynamics* (QCD) is an area of theoretical particle physics in which the strong interaction between quarks is studied. In *lattice QCD*, this theory is discretized and simulated on a four-dimensional space–time lattice with 12 variables at each lattice point, each corresponding to combinations of three colors and four spins. The action of (Stieltjes) matrix functions on vectors arises at various places in lattice QCD simulations. One such application is the *rational hybrid Monte Carlo (RHMC)* algorithm; see, e.g., [22]. In this algorithm, one needs to approximate

$$(M^H M)^{1/k}\boldsymbol{b} \text{ with } M = I - \kappa D,$$

where $k \geq 2$ is a positive integer, $\boldsymbol{b}$ is a random vector, $D$ represents a periodic nearest-neighbor coupling on the lattice, and $\kappa$ is a parameter chosen smaller than a "critical value" $\kappa_{\text{crit}}$. The matrix $M^H M$ is HPD and $f(z) = z^{1/k}$, while not a Stieltjes

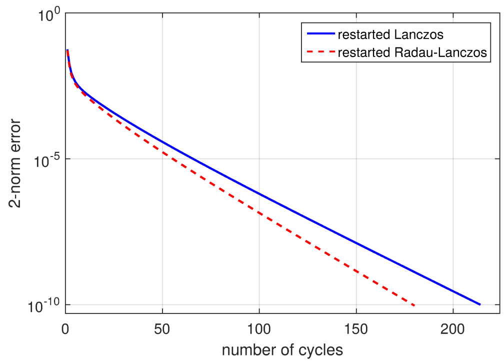


FIG. 5. *Convergence history of the Lanczos and Radau–Lanczos method for approximating* $(M^HM)^{-3/4}M^HM\boldsymbol{b}$ *for a lattice QCD model problem on an* $8^4$ *lattice, with restart parameter* $m$=10.

TABLE 2
*Improvement of the restarted Radau–Lanczos method over the standard restarted Lanczos method for the RHMC model problem for varying restart length* $m$.

| $m$ | 2 | 5 | 10 | 20 | 30 |
|---|---|---|---|---|---|
| % reduction of restart cycles | 52.12% | 29.0% | 15.9% | 8.5% | 3.3% |

function, can be rewritten as $zz^{1/k-1}$, so that $f(M^HM)\boldsymbol{b}$ can be computed as $\widetilde{f}(A)\widetilde{\boldsymbol{b}}$, where $\widetilde{f}(z) = z^{1/k-1}$ and $\widetilde{b} = M^HM\boldsymbol{b}$, making our theory applicable to this situation. We briefly mention that it is also possible to extend our theory to general functions of the type $z\widetilde{f}(z)$, analogously to [10, Corollary 3.6], thus avoiding the premultiplication of the vector $\boldsymbol{b}$ by $M^HM$, but details on this are beyond the scope of this paper. For our experiment, we choose a problem coming from an $8 \times 8 \times 8 \times 8$ lattice, resulting in a matrix of size 49,152 $\times$ 49,152, and approximate $(M^HM)^{1/4}\boldsymbol{b}$ by applying the Lanczos and Radau–Lanczos methods to $(M^HM)^{-3/4}\widetilde{\boldsymbol{b}}$. The results for our default set of parameters are presented in Figure 5, again showing a similar behavior to that observed in the previous experiments.

In addition to the above experiment, we also use the RHMC model problem to study the influence of the restart length on the convergence acceleration of the Radau–Lanczos method over the standard Lanczos method. Table 2 depicts the percentage reduction in cycles of the Radau–Lanczos method for different restart lengths. The results of these experiments confirm our explanation of the superiority of the Radau–Lanczos method given in section 4. The larger the restart length $m$, the better the approximation quality of the largest Ritz value in the standard Lanczos method, so that the acceleration of the Radau–Lanczos method is not so significant in these cases. Still, we observe that the Radau–Lanczos method outperforms the standard one for all tested restart lengths. It is especially attractive, however, when a very small restart length has to be used due to scarce memory.

**6. Conclusions.** We have presented an acceleration technique for the restarted Lanczos method for $f(A)\boldsymbol{b}$, based on a rank-one modification of the tridiagonal matrix $T_m$ related to the Gauss–Radau quadrature rule. We have developed a theory for rank-one modifications of the Lanczos method in general, but particularly analyzed the convergence of the Radau–Lanczos method and investigated its properties in various numerical experiments. Our observations indicate that the method performs better than the standard Lanczos method in situations where memory is scarce and one therefore has to resort to short cycle lengths. We have seen that the Radau–Lanczos method can mitigate the slow convergence caused by unsatisfactory convergence of the largest Ritz value to the largest eigenvalue, which occurs in the standard Lanczos method. While the Radau–Lanczos method requires knowledge of an upper bound for the largest eigenvalue of $A$ to do so, we stress that it is still preferable over the standard Lanczos method in many cases, e.g., when analytic bounds for the spectrum are known from knowledge of properties of an underlying model. We have also illustrated that the Radau–Lanczos method is robust with respect to the approximation of the largest eigenvalue, so that a rough estimate of $\lambda_{\max}$ is often sufficient, as long as it is an upper bound.

We did not discuss behavior in floating-point arithmetic in detail, but the Radau–Lanczos method can be expected to exhibit the same behavior as the standard restarted Lanczos method, which works well in practice even though the orthogonality of the Lanczos vectors may be lost. The additional operations introduced by the Radau modification are not prone to numerical instabilities. As the new method is particularly attractive in situations where small restart lengths are to be used, loss of orthogonality of the Lanczos basis is typically even less of an issue. We also refer to [11, section 6.2], where the behavior of the Gauss–Radau rank-one modification in floating-point arithmetic is investigated in the context of computing error bounds in the Lanczos method.

Another technique aimed at accelerating convergence for slowly converging restarted methods is the deflated restart approach. However, as this technique relies on Ritz value information, it often does not drastically improve the convergence behavior in situations where the Ritz values do not approximate the target eigenvalues well. Our approach can thus be seen as an alternative to deflated restarting and is successfully applicable in situations where deflated restarts are not, as demonstrated by the strong convergence results presented in this paper.

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## REFERENCES

[1] M. Afanasjew, M. Eiermann, O. G. Ernst, and S. Güttel, *Implementation of a restarted Krylov subspace method for the evaluation of matrix functions*, Linear Algebra Appl., 429 (2008), pp. 229–314.

[2] M. Benzi, E. Estrada, and C. Klymko, *Ranking hubs and authorities using matrix functions*, Linear Algebra Appl., 438 (2013), pp. 2447–2474.

[3] J. C. R. Bloch, A. Frommer, B. Lang, and T. Wettig, *An iterative method to compute the sign function of a non-Hermitian matrix and its application to the overlap Dirac operator at nonzero chemical potential*, Comput. Phys. Commun., 177 (2007), pp. 933–943.

[4] V. Druskin and L. Knizhnerman, *Extended Krylov subspaces: Approximation of the matrix square root and related functions*, SIAM J. Matrix Anal. Appl., 19 (1998), pp. 755–771.

[5] M. Eiermann and O. G. Ernst, *A restarted Krylov subspace method for the evaluation of matrix functions*, SIAM J. Numer. Anal., 44 (2006), pp. 2481–2504.

[6] M. Eiermann, O. G. Ernst, and S. Güttel, *Deflated restarting for matrix functions*, SIAM J. Matrix Anal. Appl., 32 (2011), pp. 621–641.

[7] J. v. Eshof, A. Frommer, T. Lippert, K. Schilling, and H. A. v. Vorst, *Numerical methods for the QCD overlap operator. I. Sign-function and error bounds*, Comput. Phys. Commun., 146 (2002), pp. 203–224.

[8] E. Estrada and D. J. Higham, *Network properties revealed through matrix functions*, SIAM Rev., 52 (2010), pp. 696–714.

[9] A. Frommer, S. Güttel, and M. Schweitzer, *Convergence of restarted Krylov subspace methods for Stieltjes functions of matrices*, SIAM J. Matrix Anal. Appl., 35 (2014), pp. 1602–1624.
[10] A. Frommer, S. Güttel, and M. Schweitzer, *Efficient and stable Arnoldi restarts for matrix functions based on quadrature*, SIAM J. Matrix Anal. Appl., 35 (2014), pp. 661–683.
[11] A. Frommer and M. Schweitzer, *Error bounds and estimates for Krylov subspace approximations of Stieltjes matrix functions*, BIT, 56 (2016), pp. 865–892.
[12] W. Gautschi, *Gauss-Radau formulae for Jacobi and Laguerre weight functions*, Math. Comput. Simulation, 54 (2000), pp. 403–412.
[13] G. H. Golub, *Some modified matrix eigenvalue problems*, SIAM Rev., 15 (1973), pp. 318–334.
[14] G. H. Golub and G. Meurant, *Matrices, Moments and Quadrature with Applications*, Princeton University Press, Princeton, NJ, 2010.
[15] S. Goossens and D. Roose, *Ritz and harmonic Ritz values and the convergence of FOM and GMRES*, Numer. Linear Algebra Appl., 6 (1999), pp. 281–293.
[16] P. Henrici, *Applied and Computational Complex Analysis, Vol.* 2, Wiley, New York, 1977.
[17] N. J. Higham, *Functions of Matrices: Theory and Computation*, SIAM, Philadelphia, 2008.
[18] M. Hochbruck and C. Lubich, *On Krylov subspace approximations to the matrix exponential operator*, SIAM J. Numer. Anal., 34 (1997), pp. 1911–1925.
[19] M. Hochbruck, C. Lubich, and H. Selhofer, *Exponential integrators for large systems of differential equations*, SIAM J. Sci. Comput., 19 (1998), pp. 1552–1574.
[20] M. Hochbruck and A. Ostermann, *Exponential integrators*, Acta Numerica, 19 (2010), pp. 209–286.
[21] M. Ilić, I. W. Turner, and D. P. Simpson, *A restarted Lanczos approximation to functions of a symmetric matrix*, IMA J. Numer. Anal., 30 (2010), pp. 1044–1061.
[22] A. D. Kennedy, *Algorithms for dynamical fermions*, preprint, arXiv:hep-lat/0607038v1, 2006.
[23] D. G. Luenberger, *Linear and Nonlinear Programming*, 2nd ed., Adison-Wesley, Reading, MA, 1984.
[24] C. C. Paige, B. N. Parlett, and H. A. v. Vorst, *Approximate solutions and eigenvalue bounds from Krylov subspaces*, Numer. Linear Algebra Appl., 2 (1995), pp. 115–133.
[25] Y. Saad, *Analysis of some Krylov subspace approximations to the matrix exponential operator*, SIAM J. Numer. Anal., 29 (1992), pp. 209–228.
[26] Y. Saad, *Iterative Methods for Sparse Linear Systems*, 2nd ed., SIAM, Philadelphia, 2003.
[27] D. P. Simpson, *Krylov Subspace Methods for Approximating Functions of Symmetric Positive Definite Matrices with Applications to Applied Statistics and Anomalous Diffusion*, PhD thesis, School of Mathematical Sciences, Queensland University of Technology, Brisbane, Australia, 2008.