

MODIFIED RECYCLING MINRES WITH APPLICATION TO NONLINEAR SCHRÖDINGER PROBLEMS

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Abstract. The authors propose a recycling MINRES scheme for a solution of subsequent self-adjoint linear systems as appearing, for example, in the Newton process for solving nonlinear equations. Ritz vectors are automatically extracted from one MINRES run and then used for self-adjoint deflation in the next. The method is designed to work with a preconditioner and arbitrary inner products. Numerical experiments with nonlinear Schrödinger equations indicate a substantial decrease in computation time when recycling is used.

Key words. Krylov subspace methods, MINRES, deflation, Ritz vector recycling, nonlinear Schrödinger equations, Ginzburg–Landau equations

AMS subject classifications. 65F10, 65F08, 35Q55, 35Q56

1. Introduction. Sequences of linear algebraic systems frequently occur in the numerical solution process of various kinds of problems. Most notable are implicit time stepping schemes and Newton’s method for solving nonlinear equation systems. It is often the case that the operators in subsequent linear systems have similar spectral properties or are in fact equal. To exploit this, a common approach is to factorize the operator once and apply the factorization to the following steps. However, this strategy typically has high memory requirements and is thus hardly applicable to problems with many unknowns. Also, it is not applicable if subsequent linear operators are even only slightly different from each other.

The authors use the idea of an alternative approach that carries over spectral information from one linear system to the next by extracting approximations of eigenvectors and using them in a deflation framework [18, 2, 27, 19]. For a more detailed overview on the background of such methods, see [8]. The method is designed for Krylov subspace methods in general and is worked out in this paper for the MINRES method [24] in particular. This is motivated by the fact that all observables of quantum-dynamical systems are self-adjoint.

The idea of recycling spectral information in Krylov subspace methods is not new. Notably, Wang, de Sturler, and Paulino proposed the RMINRES method [36] that includes the extraction of approximate eigenvectors, i.e., Ritz vectors and a modification of the MINRES method that includes these vectors in the search space for the following linear systems (*augmentation*). The RMINRES method with augmentation of the search space is mathematically equivalent to the standard MINRES method applied to a projected linear system [8]. Krylov subspace methods that are applied to projected linear systems are often called *deflated* methods. In literature, both augmented and deflated methods have been used in a variety of settings; we refer to the review article by Simoncini and Szyld [31] for a comprehensive overview.

The method proposed here differs from RMINRES in that it preserves self-adjointness and allows for arbitrary preconditioners and inner products (see sec-

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tion 2.2). As an added benefit, the approach can also incorporate spectral information that is explicitly provided. This is of particular interest for problems which are known to have a small number of eigenvalues that harm the the Krylov convergence, e.g., eigenvalues of large or small magnitude. An important field of application here are nonlinear problems that bear some kind of continuous symmetry, e.g., gauge invariance [17]. Even if distinctly definite, linearizations of these problems around any nontrivial solution typically have a nontrivial null space, i.e., one or more eigenvalues which are exactly 0.

As a landmark example for this class of problems, we will consider nonlinear Schrödinger equations. Nonlinear Schrödinger equations and their variations are used to describe a wide variety of physical systems, most notably in superconductivity, quantum condensates, nonlinear acoustics [34], nonlinear optics [10], and hydrodynamics [22]. Although the existence of steady state solutions is proven in certain cases, analytic expressions for realistic systems are often impossible to obtain. Hence, numerical solution methods are of particular importance for gaining insight in the physics of the system. For the solution of nonlinear Schrödinger equations with Newton's method, a linear system has to be solved with the Jacobian operator for each Newton update. The Jacobian operator is self-adjoint with respect to a nonstandard inner product which renders most default approaches unusable. In general, the Jacobian operator is indefinite and thus the MINRES method with the appropriate inner product is a suitable choice for solving the occurring linear systems. In order to be applicable in practice, the MINRES method has to be combined with a preconditioner that is able to limit the number of MINRES iterations to a feasible extent [29]. Due to the special structure of the nonlinear Schrödinger equation, the Jacobian operator exhibits one eigenvalue that moves to zero when the Newton iterate converges to a nontrivial solution and is exactly zero in a solution. Because this situation only occurs in the last step, no linear system has to be solved with an exactly singular Jacobian operator but the severely ill-conditioned Jacobian operators in the final Newton steps lead to convergence slowdown or stagnation in the MINRES method even when a preconditioner is applied. One important instance of nonlinear Schrödinger equations is the Ginzburg–Landau equation that models phenomena of certain superconductors. We propose a recycling MINRES method and show how it can help to improve the convergence of the MINRES method and thus the overall time consumption of Newton's method for the Ginzburg–Landau equation.

The paper is organized as follows: section 2 gives a brief overview on the preconditioned MINRES method for an arbitrary nonsingular linear operator that is self-adjoint with respect to an arbitrary inner product. The deflated MINRES method is described in subsection 2.2 while subsection 2.3 presents the computation of Ritz vectors and explains their use in the overall algorithm for the solution of a sequence of self-adjoint linear systems. In section 3 this algorithm is applied to the Ginzburg–Landau equation. Subsections 3.1 and 3.2 deal with the numerical treatment of nonlinear Schrödinger equations in general and the Ginzburg–Landau equation in particular. In subsection 3.3 numerical results for typical two- and three-dimensional setups are presented.

2. MINRES.

2.1. Preconditioned MINRES with arbitrary inner product. This section presents well-known properties of the preconditioned MINRES method. As opposed to ordinary textbook presentations this section incorporates a general Hilbert space. For $\mathbb{K} \in \{\mathbb{R}, \mathbb{C}\}$ let H be a \mathbb{K} -Hilbert space with inner product $\langle \cdot, \cdot \rangle_H$ and

induced norm $\|\cdot\|_H$. Throughout this paper the inner product $\langle \cdot, \cdot \rangle_H$ is linear in the first and anti-linear in the second argument and we define $L(H) := \{\mathcal{L} : H \rightarrow H \mid \mathcal{L} \text{ is linear and bounded}\}$. We wish to obtain $x \in H$ from

$$\mathcal{A}x = b \quad (2.1)$$

where $\mathcal{A} \in L(H)$ is $\langle \cdot, \cdot \rangle_H$ -self-adjoint and invertible and $b \in H$. The self-adjointness implies that the spectrum $\sigma(\mathcal{A})$ is real. However, we do not assume that \mathcal{A} is definite.

If an initial guess $x_0 \in H$ is given, we can approximate x by iterates

$$x_n = x_0 + y_n \quad \text{with} \quad y_n \in \mathcal{K}_n(\mathcal{A}, r_0) \quad (2.2)$$

where $r_0 = b - \mathcal{A}x_0$ is the initial residual and $\mathcal{K}_n(\mathcal{A}, r_0) = \text{span}\{r_0, \mathcal{A}r_0, \dots, \mathcal{A}^{n-1}r_0\}$ is the n th Krylov subspace generated with \mathcal{A} and r_0 . We concentrate on minimal residual methods here, i.e., methods that construct iterates of the form (2.2) such that the residual $r_n := b - \mathcal{A}x_n$ has minimal $\|\cdot\|_H$ -norm, that is

$$\begin{aligned} \|r_n\|_H &= \|b - \mathcal{A}x_n\|_H = \|b - \mathcal{A}(x_0 + y_n)\|_H = \|r_0 - \mathcal{A}y_n\|_H \\ &= \min_{y \in \mathcal{K}_n(\mathcal{A}, r_0)} \|r_0 - \mathcal{A}y\|_H = \min_{p \in \Pi_n^0} \|p(\mathcal{A})r_0\|_H \end{aligned} \quad (2.3)$$

where Π_n^0 is the set of polynomials of degree at most n with $p(0) = 1$. For a general invertible linear operator \mathcal{A} , the minimization problem in (2.3) can be solved by the GMRES method [26] which is equivalent to the MINRES method [24] if \mathcal{A} is self-adjoint because then the Lanczos algorithm can be used to obtain a $\langle \cdot, \cdot \rangle_H$ -orthonormal basis of the Krylov subspace $\mathcal{K}_n(\mathcal{A}, r_0)$.

To facilitate subsequent definitions and statements for general Hilbert spaces, we use a block notation for inner products that generalizes the common block notation for matrices:

DEFINITION 2.1. For $k, l \in \mathbb{N}$ and two tuples of vectors $X = [x_1, \dots, x_k] \in H^k$ and $Y = [y_1, \dots, y_l] \in H^l$ the block inner product $\langle \cdot, \cdot \rangle_H : H^k \times H^l \rightarrow \mathbb{K}^{k,l}$ is defined by

$$\langle X, Y \rangle_H := [\langle x_i, y_j \rangle_H]_{\substack{i=1, \dots, k \\ j=1, \dots, l}}.$$

A block $X \in H^k$ can be right-multiplied with a matrix just as in the plain matrix case:

DEFINITION 2.2. For $X \in H^k$ and $\mathbf{Z} = [z_{ij}]_{\substack{i=1, \dots, k \\ j=1, \dots, l}} \in \mathbb{K}^{k,l}$, right multiplication is defined by

$$X\mathbf{Z} := \left[\sum_{i=1}^k z_{ij}x_i \right]_{j=1, \dots, l} \in H^l.$$

Because the MINRES method and the underlying Lanczos algorithm is often stated for Hermitian matrices only (i.e., for the Euclidean inner product), we recall very briefly some properties of the Lanczos algorithm for a linear operator that is self-adjoint with respect to an arbitrary inner product $\langle \cdot, \cdot \rangle_H$. If the Lanczos algorithm with inner product $\langle \cdot, \cdot \rangle_H$ applied to \mathcal{A} and the initial vector $v_1 = r_0 / \|r_0\|_H$ has completed the n th iteration, the Lanczos relation

$$\mathcal{A}V_n = V_{n+1}\mathbf{T}_n \quad (2.4)$$

holds, where the elements of $V_{n+1} = [v_1, \dots, v_{n+1}] \in H^{n+1}$ form a $\langle \cdot, \cdot \rangle_H$ -orthonormal basis of $\mathcal{K}_{n+1}(\mathcal{A}, r_0)$, i.e., $\text{span}\{v_1, \dots, v_{n+1}\} = \mathcal{K}_{n+1}(\mathcal{A}, r_0)$ and $\langle V_{n+1}, V_{n+1} \rangle_H = \mathbf{I}_{n+1}$. The matrix $\underline{\mathbf{T}}_n \in \mathbb{R}^{n+1, n}$ is real-valued (even if $\mathbb{K} = \mathbb{C}$), symmetric, and tridiagonal with

$$\underline{\mathbf{T}}_k = [\langle \mathcal{A}v_i, v_j \rangle_H]_{\substack{i=1, \dots, n+1 \\ j=1, \dots, n}}.$$

The n th approximation of the solution of the linear system (2.1) generated with the MINRES method and the corresponding residual norm, cf. (2.2) and (2.3), can then be expressed as

$$\begin{aligned} x_n &= x_0 + V_n z_n \quad \text{with } z_n \in \mathbb{K}^n \quad \text{and} \\ \|r_n\|_H &= \|r_0 - \mathcal{A}V_n z_n\|_H = \|V_{n+1}(\|r_0\|_H e_1 - \underline{\mathbf{T}}_n z_n)\|_H = \|\|r_0\|_H e_1 - \underline{\mathbf{T}}_n z_n\|_2. \end{aligned}$$

By iteratively computing a QR decomposition of $\underline{\mathbf{T}}_n$, the minimization problem in (2.3) can be solved without storing the full matrix $\underline{\mathbf{T}}_n$ and, more importantly, the full Lanczos basis V_n .

If $N := \dim H < \infty$ and the elements of $U \in H^N$ form a $\langle \cdot, \cdot \rangle_H$ -orthonormal eigenvector basis of H , then $\mathcal{A}U = U\mathbf{D}$ for the diagonal matrix $\mathbf{D} = \text{diag}(\lambda_1, \dots, \lambda_N)$ with \mathcal{A} 's eigenvalues $\lambda_1, \dots, \lambda_N \in \mathbb{R}$ on the diagonal. Let $r_0^U \in \mathbb{K}^N$ be the representation of r_0 in the basis U , i.e., $r_0 = Ur_0^U$. According to (2.3), the residual norm of the n th approximation obtained with MINRES can be expressed as

$$\begin{aligned} \|r_n\|_H &= \min_{p \in \Pi_n^0} \|p(\mathcal{A})Ur_0^U\|_H = \min_{p \in \Pi_n^0} \|Up(\mathbf{D})r_0^U\|_H = \min_{p \in \Pi_n^0} \|p(\mathbf{D})r_0^U\|_2 \\ &\leq \|r_0^U\|_2 \min_{p \in \Pi_n^0} \|p(\mathbf{D})\|_2. \end{aligned} \quad (2.5)$$

From $\|r_0^U\|_2 = \|Ur_0^U\|_H = \|r_0\|_H$ and $\|p(\mathbf{D})\|_2 = \max_{i \in \{1, \dots, N\}} |p(\lambda_i)|$, we obtain the well-known MINRES worst-case bound for the relative residual norm [12, 15]

$$\frac{\|r_n\|_H}{\|r_0\|_H} \leq \min_{p \in \Pi_n^0} \max_{i \in \{1, \dots, N\}} |p(\lambda_i)|. \quad (2.6)$$

This can be estimated even further upon letting the eigenvalues of \mathcal{A} be sorted such that $\lambda_1 \leq \dots \leq \lambda_s < 0 < \lambda_{s+1} \leq \dots \leq \lambda_N$ for a $s \in \mathbb{N}_0$. By replacing the discrete set of eigenvalues in (2.6) by the union of the two intervals $I^- := [\lambda_1, \lambda_s]$ and $I^+ := [\lambda_{s+1}, \lambda_N]$, one gets

$$\begin{aligned} \frac{\|r_n\|_H}{\|r_0\|_H} &\leq \min_{p \in \Pi_n^0} \max_{i \in \{1, \dots, N\}} |p(\lambda_i)| \leq \min_{p \in \Pi_n^0} \max_{\lambda \in I^- \cup I^+} |p(\lambda)| \\ &\leq 2 \left(\frac{\sqrt{|\lambda_1 \lambda_N|} - \sqrt{|\lambda_s \lambda_{s+1}|}}{\sqrt{|\lambda_1 \lambda_N|} + \sqrt{|\lambda_s \lambda_{s+1}|}} \right)^{[n/2]}, \end{aligned} \quad (2.7)$$

where $[n/2]$ is the integer part of $n/2$, cf. [12, 15]. Note that this estimate does not take into account the actual distribution of the eigenvalues in the intervals I^- and I^+ . In practice a better convergence behavior than the one suggested by the estimate above can often be observed.

In most applications, the MINRES method is only feasible when it is applied with a preconditioner. Consider the preconditioned system

$$\mathcal{M}^{-1}\mathcal{A}x = \mathcal{M}^{-1}b \quad (2.8)$$

where $\mathcal{M} : H \rightarrow H$ is a $\langle \cdot, \cdot \rangle_H$ -self-adjoint, invertible, and positive-definite linear operator. Note that $\mathcal{M}^{-1}\mathcal{A}$ is not $\langle \cdot, \cdot \rangle_H$ -self-adjoint but self-adjoint with respect to the inner product $\langle \cdot, \cdot \rangle_{\mathcal{M}}$ defined by $\langle x, y \rangle_{\mathcal{M}} := \langle \mathcal{M}x, y \rangle_H = \langle x, \mathcal{M}y \rangle_H$. The MINRES method is then applied to (2.8) with the inner product $\langle \cdot, \cdot \rangle_{\mathcal{M}}$ and thus minimizes $\|\mathcal{M}^{-1}b - \mathcal{M}^{-1}\mathcal{A}x\|_{\mathcal{M}}$. From an algorithmic point of view it is worthwhile to note that only the application of \mathcal{M}^{-1} is needed and the application of \mathcal{M} for the inner products can be carried out implicitly; cf. [7, chapter 6]. The convergence bound in (2.7) then refers to the eigenvalues of $\mathcal{M}^{-1}\mathcal{A}$ and the goal of preconditioning is to achieve a more favorable spectrum of $\mathcal{M}^{-1}\mathcal{A}$ with an appropriate \mathcal{M}^{-1} .

2.2. Deflated MINRES. In many applications even with the aid of a preconditioner the convergence of MINRES is hampered – often due to the presence of one or a few eigenvalues close to zero that are isolated from the remaining spectrum. This case has recently been studied by Simoncini and Szyld [32]. Their analysis and numerical experiments show that an isolated simple eigenvalue can cause stagnation of the residual norm until a harmonic Ritz value approximates the outlying eigenvalue well.

Two strategies are well-known in the literature to circumvent the stagnation or slowdown in the convergence of preconditioned Krylov subspace methods described above: *augmentation* and *deflation*. In augmented methods the Krylov subspace is enlarged by a suitable subspace that contains useful information about the problem. In deflation techniques the operator is modified with a suitably chosen projection in order to “eliminate” components that hamper convergence (e.g., eigenvalues close to the origin). For an extensive overview of these techniques we refer to the survey article by Simoncini and Szyld [31]. Both techniques are closely intertwined and even turn out to be equivalent in some cases [8]. Here, we concentrate on deflated methods and first give a brief description of the recycling MINRES (RMINRES) method introduced by Wang, de Sturler, and Paulino [36] before presenting a slightly different approach.

The RMINRES method by Wang, de Sturler, and Paulino [36] is mathematically equivalent [8] to the application of the MINRES method to the “deflated” equation

$$\mathcal{P}_1\mathcal{A}\tilde{x} = \mathcal{P}_1b \quad (2.9)$$

where for a given k -tuple $U \in H^k$ of linearly independent vectors (which constitute a basis of the “recycled” space) and $C := \mathcal{A}U$, the linear operator $\mathcal{P}_1 : H \rightarrow H$ is defined by $\mathcal{P}_1x := x - C\langle C, C \rangle_H^{-1}\langle C, x \rangle_H$ for an arbitrary inner product. Note that, although \mathcal{P}_1 is a $\langle \cdot, \cdot \rangle$ -self-adjoint projection, $\mathcal{P}_1\mathcal{A}$ in general is not. However, as outlined in [36, section 4] an orthonormal basis of the Krylov subspace can still be generated with MINRES’ short recurrences and the operator $\mathcal{P}_1\mathcal{A}$ because $\mathcal{K}_n(\mathcal{P}_1\mathcal{A}, \mathcal{P}_1r_0) = \mathcal{K}_n(\mathcal{P}_1\mathcal{A}\mathcal{P}_1^*, \mathcal{P}_1r_0)$. Solutions of equation (2.9) are not unique for $k > 0$ and thus x was replaced by \tilde{x} . To obtain an approximation x_n of the original solution x from the approximation \tilde{x}_n generated with MINRES applied to (2.9), an additional correction has to be applied:

$$x_n = \tilde{\mathcal{P}}_1\tilde{x}_n + U\langle C, C \rangle_H^{-1}\langle C, b \rangle_H,$$

where $\tilde{\mathcal{P}}_1 : H \rightarrow H$ is defined by $\tilde{\mathcal{P}}_1x := x - U\langle C, C \rangle_H^{-1}\langle C, \mathcal{A}x \rangle_H$. As outlined in [8, section 5], the RMINRES method may suffer from breakdowns which can be cured by using the adapted initial guess $\tilde{x}_0 := \tilde{\mathcal{P}}_1x_0 + C\langle C, C \rangle_H^{-1}\langle U, b \rangle_H$.

Let us now turn to a slightly different deflation technique for MINRES which we formulate with preconditioning directly. We will use a projection which has been

developed in the context of the CG method for Hermitian and positive-definite operators [21, 3, 35]. Under a mild assumption, this projection can also be used in the indefinite case with the MINRES method. Our goal is to use approximations to eigenvectors corresponding to eigenvalues that hamper convergence in order to modify the operator with a projection. Consider the preconditioned equation (2.8) and assume for a moment that the elements of $U = [u_1, \dots, u_k] \in H^k$ form a $\langle \cdot, \cdot \rangle_{\mathcal{M}}$ -orthonormal basis consisting of eigenvectors of $\mathcal{M}^{-1}\mathcal{A}$, i.e., $\mathcal{M}^{-1}\mathcal{A}U = U\mathbf{D}$ with a diagonal matrix $\mathbf{D} = \text{diag}(\lambda_1, \dots, \lambda_k) \in \mathbb{R}^{k,k}$. Then $\langle U, \mathcal{M}^{-1}\mathcal{A}U \rangle_{\mathcal{M}} = \langle U, U \rangle_{\mathcal{M}}\mathbf{D} = \mathbf{D}$ is nonsingular because we assumed that \mathcal{A} is invertible. This motivates the following definition:

DEFINITION 2.3. *Let $\mathcal{M}, \mathcal{A} \in L(H)$ be invertible and $\langle \cdot, \cdot \rangle_H$ -self-adjoint operators with positive-definite \mathcal{M} . Let $U \in H^k$ be such that $\langle U, \mathcal{M}^{-1}\mathcal{A}U \rangle_{\mathcal{M}} = \langle U, \mathcal{A}U \rangle_H$ is nonsingular. We define the projections $\mathcal{P}_{\mathcal{M}}, \mathcal{P} : H \rightarrow H$ by*

$$\begin{aligned} \mathcal{P}_{\mathcal{M}}x &:= x - \mathcal{M}^{-1}\mathcal{A}U\langle U, \mathcal{M}^{-1}\mathcal{A}U \rangle_{\mathcal{M}}^{-1}\langle U, x \rangle_{\mathcal{M}} \\ \mathcal{P}x &:= x - \mathcal{A}U\langle U, \mathcal{A}U \rangle_H^{-1}\langle U, x \rangle_H. \end{aligned} \quad (2.10)$$

The assumption in definition 2.3 that $\langle U, \mathcal{M}^{-1}\mathcal{A}U \rangle_{\mathcal{M}}$ is nonsingular holds if and only if $\text{range}(\mathcal{M}^{-1}\mathcal{A}U) \cap \text{range}(U)^{\perp_{\mathcal{M}}} = \{0\}$ or equivalently if $\text{range}(\mathcal{A}U) \cap \text{range}(U)^{\perp_H} = \{0\}$ which is fulfilled for good-enough approximations of eigenvectors. Applying the projection $\mathcal{P}_{\mathcal{M}}$ to the preconditioned equation (2.8) yields the deflated equation

$$\mathcal{P}_{\mathcal{M}}\mathcal{M}^{-1}\mathcal{A}\tilde{x} = \mathcal{P}_{\mathcal{M}}\mathcal{M}^{-1}b. \quad (2.11)$$

The following lemma states some important properties of the operator $\mathcal{P}_{\mathcal{M}}\mathcal{M}^{-1}\mathcal{A}$.

LEMMA 2.4. *Let the assumptions in definition 2.3 hold. Then*

1. $\mathcal{P}_{\mathcal{M}}\mathcal{M}^{-1} = \mathcal{M}^{-1}\mathcal{P}$.
2. $\mathcal{P}\mathcal{A} = \mathcal{A}\mathcal{P}^*$ where \mathcal{P}^* is the adjoint operator of \mathcal{P} with respect to $\langle \cdot, \cdot \rangle_H$, defined by $\mathcal{P}^*x = x - U\langle U, \mathcal{A}U \rangle_H^{-1}\langle \mathcal{A}U, x \rangle_H$.
3. $\mathcal{P}_{\mathcal{M}}\mathcal{M}^{-1}\mathcal{A} = \mathcal{M}^{-1}\mathcal{P}\mathcal{A} = \mathcal{M}^{-1}\mathcal{A}\mathcal{P}^*$ is self-adjoint with respect to $\langle \cdot, \cdot \rangle_{\mathcal{M}}$.
4. For each initial guess $\tilde{x}_0 \in H$, the MINRES method with inner product $\langle \cdot, \cdot \rangle_{\mathcal{M}}$ applied to equation (2.11) is well defined at each iteration until it terminates with a solution of the system.
5. If \tilde{x}_n is the n th approximation and $\mathcal{P}_{\mathcal{M}}\mathcal{M}^{-1}b - \mathcal{P}_{\mathcal{M}}\mathcal{M}^{-1}\mathcal{A}\tilde{x}_n$ the corresponding residual generated by the MINRES method with inner product $\langle \cdot, \cdot \rangle_{\mathcal{M}}$ applied to (2.11) with initial guess $\tilde{x}_0 \in H$, then the corrected approximation

$$x_n := \mathcal{P}^*\tilde{x}_n + U\langle U, \mathcal{A}U \rangle_H^{-1}\langle U, b \rangle_H \quad (2.12)$$

fulfills

$$\mathcal{M}^{-1}b - \mathcal{M}^{-1}\mathcal{A}x_n = \mathcal{P}_{\mathcal{M}}\mathcal{M}^{-1}b - \mathcal{P}_{\mathcal{M}}\mathcal{M}^{-1}\mathcal{A}\tilde{x}_n. \quad (2.13)$$

(Note that (2.13) also holds for $n = 0$.)

Proof. 1., 2. and the equation in 3. follow from elementary calculations. Because

$$\begin{aligned} \langle \mathcal{P}_{\mathcal{M}}\mathcal{M}^{-1}\mathcal{A}x, y \rangle_{\mathcal{M}} &= \langle \mathcal{P}\mathcal{A}x, y \rangle_H = \langle \mathcal{A}x, \mathcal{P}^*y \rangle_H = \langle x, \mathcal{A}\mathcal{P}^*y \rangle_H = \langle x, \mathcal{P}\mathcal{A}y \rangle_H \\ &= \langle x, \mathcal{P}_{\mathcal{M}}\mathcal{M}^{-1}\mathcal{A}y \rangle_{\mathcal{M}}. \end{aligned}$$

holds for all $x, y \in H$, the operator $\mathcal{P}_{\mathcal{M}}\mathcal{M}^{-1}\mathcal{A}$ is self-adjoint with respect to $\langle \cdot, \cdot \rangle_{\mathcal{M}}$.

4. has been proved in [8, Theorem 4.1] for GMRES with the Euclidean inner product which can easily be generalized to arbitrary inner products. GMRES is mathematically equivalent to MINRES in our case due to the fact that $\mathcal{P}_M \mathcal{M}^{-1} \mathcal{A}$ is self-adjoint.

5. follows from 1. and 3. by direct calculation:

$$\begin{aligned} \mathcal{M}^{-1}b - \mathcal{M}^{-1}\mathcal{A}x_n &= \mathcal{M}^{-1}(b - \mathcal{A}U \langle U, \mathcal{A}U \rangle_H^{-1} \langle U, b \rangle_H) - \mathcal{M}^{-1}\mathcal{A}\mathcal{P}^* \tilde{x}_n \\ &= \mathcal{M}^{-1}\mathcal{P}b - \mathcal{P}_M \mathcal{M}^{-1} \mathcal{A} \tilde{x}_n = \mathcal{P}_M \mathcal{M}^{-1}b - \mathcal{P}_M \mathcal{M}^{-1} \mathcal{A} \tilde{x}_n. \end{aligned}$$

□

Now that we know that MINRES is well-defined when applied to the deflated and preconditioned equation (2.11) we want to investigate the convergence behavior in comparison to the original preconditioned equation (2.8).

LEMMA 2.5. *Let the assumptions in definition 2.3 and $N := \dim H < \infty$ hold. If $\sigma(\mathcal{M}^{-1}\mathcal{A}) = \{\lambda_1, \dots, \lambda_N\}$ is the spectrum of the preconditioned operator $\mathcal{M}^{-1}\mathcal{A}$ and for $k > 0$ the elements of $U \in H^k$ form a basis of the $\mathcal{M}^{-1}\mathcal{A}$ -invariant subspace corresponding to the eigenvalues $\lambda_1, \dots, \lambda_k$ then the following holds:*

1. *The spectrum of the deflated operator $\mathcal{P}_M \mathcal{M}^{-1} \mathcal{A}$ is*

$$\sigma(\mathcal{P}_M \mathcal{M}^{-1} \mathcal{A}) = \{0\} \cup \{\lambda_{k+1}, \dots, \lambda_N\}.$$

2. *For $n \geq 0$ let x_n be the n th corrected approximation (cf. item 5 of lemma 2.4) of MINRES applied to (2.11) with inner product $\langle \cdot, \cdot \rangle_M$ and initial guess \tilde{x}_0 . The residuals $r_n := \mathcal{M}^{-1}b - \mathcal{M}^{-1}\mathcal{A}x_n$ then fulfill*

$$\frac{\|r_n\|_M}{\|r_0\|_M} \leq \min_{p \in \Pi_n^0} \max_{i \in \{k+1, \dots, N\}} |p(\lambda_i)|. \quad (2.14)$$

Proof.

1. From the definition of \mathcal{P}_M in definition 2.3 we directly obtain $\mathcal{P}_M \mathcal{M}^{-1} \mathcal{A} U = 0$ and thus know that 0 is an eigenvalue of $\mathcal{P}_M \mathcal{M}^{-1} \mathcal{A}$ with multiplicity at least k . Let the elements of $V \in H^{N-k}$ be orthonormal and such that $\mathcal{M}^{-1} \mathcal{A} V = V \mathbf{D}_2$ with $\mathbf{D}_2 = \text{diag}(\lambda_{k+1}, \dots, \lambda_N)$. Then $\langle U, V \rangle_M = 0$ because $\mathcal{M}^{-1} \mathcal{A}$ is self-adjoint with respect to $\langle \cdot, \cdot \rangle_M$. Thus $\mathcal{P}_M V = V$ and the statement follows from $\mathcal{P}_M \mathcal{M}^{-1} \mathcal{A} V = V \mathbf{D}_2$.
2. Because the residual corresponding to the corrected initial guess is $r_0 = \mathcal{P}_M \mathcal{M}^{-1}(b - \mathcal{A} \tilde{x}_0) \in \text{range}(U)^\perp = \text{range}(V)$, where V is defined as in 1., we have $r_0 = V r_0^V$ for a $r_0^V \in \mathbb{K}^{N-k}$. Then with \mathbf{D}_2 as in 1. we obtain by using the orthonormality of V similar to (2.5):

$$\begin{aligned} \|r_n\|_M &= \min_{p \in \Pi_n^0} \|p(\mathcal{P}_M \mathcal{M}^{-1} \mathcal{A}) V r_0^V\|_M = \min_{p \in \Pi_n^0} \|V p(\mathbf{D}_2) r_0^V\|_M = \min_{p \in \Pi_n^0} \|p(\mathbf{D}_2) r_0^V\|_2 \\ &\leq \|r_0\|_M \min_{p \in \Pi_n^0} \max_{i \in \{k+1, \dots, N\}} |p(\lambda_i)|. \end{aligned}$$

□

Implementational notes. Item 1 of lemma 2.4 states that $\mathcal{P}_M \mathcal{M}^{-1} = \mathcal{M}^{-1} \mathcal{P}$ and thus the MINRES method can be applied to the linear system

$$\mathcal{M}^{-1} \mathcal{P} \mathcal{A} \tilde{x} = \mathcal{M}^{-1} \mathcal{P} b \quad (2.15)$$

instead of (2.11). When an approximate solution \tilde{x}_n of (2.15) is satisfactory then the correction (2.12) has to be applied to obtain an approximate solution of the original

	vectors	other
U	k	–
$C = \mathcal{A}U$	k	–
$\mathbf{E} = \langle U, C \rangle_H$ or \mathbf{E}^{-1}	–	k^2

(a) Storage requirements.

	applications of \mathcal{A}	applications of \mathcal{M}^{-1}	vector updates	inner products	solve with \mathbf{E}
Construction of C and \mathbf{E}	k	–	–	$k(k+1)/2$	–
Application of \mathcal{P} or \mathcal{P}^*	–	–	k	k	1
Application of correction	–	–	k	$2k$	1

(b) Computational cost.

Table 2.1: Storage requirements and computational cost of the projection operators \mathcal{P} and \mathcal{P}^* (cf. definition 2.3 and lemma 2.4).

system (2.1). Note that neither \mathcal{M} nor its inverse \mathcal{M}^{-1} show up in the definition of the operator \mathcal{P} or its adjoint operator \mathcal{P}^* which is used in the correction. Thus the preconditioner \mathcal{M}^{-1} does not have to be applied to additional vectors if deflation is used. This can be a major advantage since the application of the preconditioner operator \mathcal{M}^{-1} is the most expensive part in many applications.

The deflation operator \mathcal{P} as defined in definition 2.3 with $U \in H^k$ needs to store $2k$ vectors because aside from U also $C := \mathcal{A}U$ should be pre-computed and stored. Furthermore the matrix $\mathbf{E} := \langle U, C \rangle_H \in \mathbb{K}^{k,k}$ or its inverse has to be stored. The adjoint operator \mathcal{P}^* needs exactly the same data so no more storage is required. The construction of C needs k applications of the operator \mathcal{A} but – as stated above – no application of the preconditioner operator \mathcal{M}^{-1} . Because \mathbf{E} is Hermitian $k(k+1)/2$ inner products have to be computed. One application of \mathcal{P} or \mathcal{P}^* requires k inner products, the solution of a linear system with the Hermitian k -by- k matrix \mathbf{E} and k vector updates. We gather this information in table 2.1.

Instead of correcting the last approximation \tilde{x}_n it is also possible to start with the corrected initial guess

$$x_0 = \mathcal{P}^* \tilde{x}_0 + U \langle U, \mathcal{A}U \rangle_H^{-1} \langle U, b \rangle_H \quad (2.16)$$

and to use \mathcal{P}^* as a right “preconditioner” (note that \mathcal{P}^* is singular in general). The difference is mainly of algorithmic nature and will be described very briefly.

For an invertible linear operator $\mathcal{B} : H \rightarrow H$ the right preconditioned system $\mathcal{A}\mathcal{B}y = b$ can be solved for y and then the original solution can be obtained from $x = \mathcal{B}y$. Instead of x_0 the initial guess $y_0 := \mathcal{B}^{-1}x_0$ is used and the initial residual $r_0 = b - \mathcal{A}\mathcal{B}y_0 = b - \mathcal{A}x_0$ equals the residual of the unpreconditioned system. Then iterates

$$y_n = y_0 + z_n \quad \text{with} \quad z_n \in \mathcal{K}_n(\mathcal{A}\mathcal{B}, r_0)$$

and $x_n := \mathcal{B}y_n = x_0 + \mathcal{B}z_n$ are constructed such that the residual $r_n = b - \mathcal{A}\mathcal{B}y_n = b - \mathcal{A}x_n$ is minimal in $\|\cdot\|_H$. If the operator $\mathcal{A}\mathcal{B}$ is self-adjoint the MINRES method can again be used to solve this minimization problem. Note that y_0 is not needed and will never be computed explicitly. The right preconditioning can of course be combined with a positive definite preconditioner as described in the introduction of section 2.

We now take a closer look at the case $\mathcal{B} = \mathcal{P}^*$ which differs from the above description because \mathcal{P}^* is not invertible in general. However, even if the right preconditioned system is not consistent (i.e., $b \notin \text{range}(\mathcal{A}\mathcal{P}^*)$) the above strategy can be used to solve the original linear system. Let us with x_0 from equation (2.16) construct iterates

$$x_n = x_0 + \mathcal{P}^*y_n \quad \text{with} \quad y_n \in \mathcal{K}_n(\mathcal{M}^{-1}\mathcal{A}\mathcal{P}^*, r_0) \quad (2.17)$$

such that the residual

$$r_n = \mathcal{M}^{-1}b - \mathcal{M}^{-1}\mathcal{A}x_n \quad (2.18)$$

has minimal $\|\cdot\|_{\mathcal{M}}$ -norm. Inserting (2.17) and the definition of x_0 into (2.18) yields $r_n = \mathcal{M}^{-1}\mathcal{P}b - \mathcal{M}^{-1}\mathcal{P}\mathcal{A}y_n$ with $y_n \in \mathcal{K}_n(\mathcal{M}^{-1}\mathcal{A}\mathcal{P}^*, r_0) = \mathcal{K}_n(\mathcal{M}^{-1}\mathcal{P}\mathcal{A}, r_0)$. The minimization problem is thus the same as in the case where MINRES is applied to the linear system (2.15) and because both the operators and initial vectors coincide the same Lanczos relation holds. Consequently the MINRES method can be applied for the right preconditioned system

$$\mathcal{M}^{-1}\mathcal{A}\mathcal{P}^*y = \mathcal{M}^{-1}b, \quad x = \mathcal{P}^*y \quad (2.19)$$

with the corrected initial guess x_0 from equation (2.16). The key issue here is that the initial guess is treated as in (2.17). A deflated and preconditioned MINRES implementation following these ideas only needs the operator \mathcal{P}^* and the corrected initial guess x_0 . A correction step at the end then is unnecessary.

2.3. Ritz vector computation. So far we considered a single linear system and assumed that a basis for the construction of the projection used in the deflated system is given (e.g. eigenvectors are given). We now turn to a sequence of preconditioned linear systems

$$\mathcal{M}_{(i)}^{-1}\mathcal{A}_{(i)}x^{(i)} = \mathcal{M}_{(i)}^{-1}b^{(i)} \quad (2.20)$$

where $\mathcal{M}_{(i)}, \mathcal{A}_{(i)} : L(H)$ are invertible and self-adjoint with respect to $\langle \cdot, \cdot \rangle_H$, $\mathcal{M}_{(i)}$ is positive definite and $x^{(i)}, b^{(i)} \in H$ for $i \in \{1, \dots, M\}$. To improve the readability we use subscript indices for operators and superscript indices for elements or tuples of the Hilbert space H . Such a sequence may arise from a time dependent problem or a nonlinear equation where solutions are approximated using Newton's method (cf. section 3). We now assume that the operator $\mathcal{M}_{(i+1)}^{-1}\mathcal{A}_{(i+1)}$ only differs slightly from the previous operator $\mathcal{M}_{(i)}^{-1}\mathcal{A}_{(i)}$. Then it may be worthwhile to extract some eigenvector approximations from the Krylov subspace *and* the deflation subspace used in the solution of the i th system in order to accelerate convergence of the next system by deflating these extracted approximate eigenvectors.

For explaining the strategy in more detail we omit the sequence index for a moment and always refer to the i th linear system if not specified otherwise. Assume that we used a tuple $U \in H^k$ whose elements form a $\langle \cdot, \cdot \rangle_{\mathcal{M}}$ -orthonormal basis

to set up the projection $\mathcal{P}_{\mathcal{M}}$ (cf. definition 2.3) for the i th linear system (2.20). We then assume that the deflated and preconditioned MINRES method with inner product $\langle \cdot, \cdot \rangle_{\mathcal{M}}$ and initial guess \tilde{x}_0 computed a satisfactory approximate solution after n steps. The MINRES method then constructed a basis of the Krylov subspace $\mathcal{K}_n(\mathcal{P}_{\mathcal{M}}\mathcal{M}^{-1}\mathcal{A}, r_0)$ where the initial residual is $r_0 = \mathcal{P}_{\mathcal{M}}\mathcal{M}^{-1}(b - \mathcal{A}\tilde{x}_0)$. Due to the definition of the projection we know that $\mathcal{K}_n(\mathcal{P}_{\mathcal{M}}\mathcal{M}^{-1}\mathcal{A}, r_0) \perp_{\mathcal{M}} \text{range}(U)$ and we now wish to compute approximate eigenvectors of $\mathcal{M}^{-1}\mathcal{A}$ in the subspace $S := \mathcal{K}_n(\mathcal{P}_{\mathcal{M}}\mathcal{M}^{-1}\mathcal{A}, r_0) \cup \text{range}(U)$. We can then pick some approximate eigenvectors according to the corresponding approximate eigenvalues and the approximation quality in order to construct a projection for the deflation of the $(i+1)$ st linear system.

Let us recall the definition of Ritz pairs [23]:

DEFINITION 2.6. *Let $S \subseteq H$ be a finite dimensional subspace and let $\mathcal{B} : H \rightarrow H$ be a linear operator. $(w, \mu) \in S \times \mathbb{C}$ is called a Ritz pair of \mathcal{B} with respect to S and the inner product $\langle \cdot, \cdot \rangle$ if*

$$\mathcal{B}w - \mu w \perp_{\langle \cdot, \cdot \rangle} S.$$

The following lemma gives insight into how the Ritz pairs of the operator $\mathcal{M}^{-1}\mathcal{A}$ with respect to the Krylov subspace $\mathcal{K}_n(\mathcal{P}_{\mathcal{M}}\mathcal{M}^{-1}\mathcal{A}, r_0)$ and the deflation subspace $\text{range}(U)$ can be obtained from data that is available when the MINRES method found a satisfactory approximate solution of the last linear system.

LEMMA 2.7. *Let $\mathcal{M}, \mathcal{A} : H \rightarrow H$ be linear, invertible, and $\langle \cdot, \cdot \rangle_H$ -self-adjoint and let \mathcal{M} be positive-definite. Furthermore, let $U \in H^k$ be such that $\langle U, U \rangle_{\mathcal{M}} = \mathbf{I}_k$ and let $\mathcal{P}_{\mathcal{M}}$ be defined as in definition 2.3.*

Assume that the Lanczos algorithm with inner product $\langle \cdot, \cdot \rangle_{\mathcal{M}}$ applied to the operator $\mathcal{P}_{\mathcal{M}}\mathcal{M}^{-1}\mathcal{A}$ and an initial vector $v \in \text{range}(U)^{\perp_{\mathcal{M}}}$ proceeds to the n th iteration and the Lanczos relation

$$\mathcal{P}_{\mathcal{M}}\mathcal{M}^{-1}\mathcal{A}V_n = V_{n+1}\mathbf{T}_n \tag{2.21}$$

holds with $V_{n+1} = [v_1, \dots, v_{n+1}] \in H^{n+1}$, $\langle V_{n+1}, V_{n+1} \rangle_{\mathcal{M}} = \mathbf{I}_{n+1}$ and $\mathbf{T}_n = \begin{bmatrix} \mathbf{T}_n & \\ 0 & \dots & 0 & s_n \end{bmatrix} \in \mathbb{R}^{n+1, n}$ where $s_n \in \mathbb{R}$ is nonnegative and $\mathbf{T}_n \in \mathbb{R}^{n, n}$ is tridiagonal, symmetric, and real-valued. Let $S := \mathcal{K}_n(\mathcal{P}_{\mathcal{M}}\mathcal{M}^{-1}\mathcal{A}, v) \cup \text{range}(U)$ and $w = [V_n, U]\tilde{w} \in S$ for a $\tilde{w} \in \mathbb{K}^{n+k}$.

Then $(w, \mu) \in S \times \mathbb{R}$ is a Ritz pair of $\mathcal{M}^{-1}\mathcal{A}$ with respect to S and the inner product $\langle \cdot, \cdot \rangle_{\mathcal{M}}$ if and only if

$$\begin{bmatrix} \mathbf{T}_n + \mathbf{B}\mathbf{E}^{-1}\mathbf{B}^H & \mathbf{B} \\ \mathbf{B}^H & \mathbf{E} \end{bmatrix} \tilde{w} = \mu \tilde{w} \tag{2.22}$$

where $\mathbf{B} := \langle V_n, \mathcal{A}U \rangle_H$ and $\mathbf{E} := \langle U, \mathcal{A}U \rangle_H$.

Furthermore, the squared $\|\cdot\|_{\mathcal{M}}$ -norm of the residual $\mathcal{M}^{-1}\mathcal{A}w - \mu w$ is

$$\|\mathcal{M}^{-1}\mathcal{A}w - \mu w\|_{\mathcal{M}}^2 = (\mathbf{G}\tilde{w})^H \begin{bmatrix} \mathbf{I}_{n+1} & \mathbf{B} & 0 \\ \mathbf{B}^H & \mathbf{F} & \mathbf{E} \\ 0 & \mathbf{E} & \mathbf{I}_k \end{bmatrix} \mathbf{G}\tilde{w} \tag{2.23}$$

where

$$\begin{aligned}\underline{\mathbf{B}} &= \langle V_{n+1}, \mathcal{A}U \rangle_H = \begin{bmatrix} \mathbf{B} \\ \langle v_{n+1}, \mathcal{A}U \rangle_H \end{bmatrix}, \\ \mathbf{F} &= \langle \mathcal{A}U, \mathcal{M}^{-1}\mathcal{A}U \rangle_H \quad \text{and} \\ \mathbf{G} &= \begin{bmatrix} \underline{\mathbf{I}}_n - \mu \underline{\mathbf{I}}_n & 0 \\ \mathbf{E}^{-1}\mathbf{B}^H & \mathbf{I}_k \\ 0 & -\mu \mathbf{I}_k \end{bmatrix} \quad \text{with} \quad \underline{\mathbf{I}}_n = \begin{bmatrix} \mathbf{I}_n \\ 0 \end{bmatrix}.\end{aligned}$$

Proof. (w, μ) is a Ritz pair of $\mathcal{M}^{-1}\mathcal{A}$ with respect to $S = \text{range}([V_n, U])$ and the inner product $\langle \cdot, \cdot \rangle_{\mathcal{M}}$ if and only if

$$\begin{aligned}& \mathcal{M}^{-1}\mathcal{A}w - \mu w \perp_{\mathcal{M}} S \\ \Leftrightarrow & \langle s, \mathcal{M}^{-1}\mathcal{A}w - \mu w \rangle_{\mathcal{M}} = 0 \quad \forall s \in S \\ \Leftrightarrow & \langle [V_n, U], (\mathcal{M}^{-1}\mathcal{A} - \mu \mathcal{I})[V_n, U] \rangle_{\mathcal{M}} \tilde{w} = 0 \\ \Leftrightarrow & \langle [V_n, U], \mathcal{M}^{-1}\mathcal{A}[V_n, U] \rangle_{\mathcal{M}} \tilde{w} = \mu \langle [V_n, U], [V_n, U] \rangle_{\mathcal{M}} \tilde{w} \\ \Leftrightarrow & \langle [V_n, U], \mathcal{M}^{-1}\mathcal{A}[V_n, U] \rangle_{\mathcal{M}} \tilde{w} = \mu \tilde{w}\end{aligned}$$

where the last equivalence follows from the orthonormality of U and V_n and the fact that $\text{range}(U) \perp_{\mathcal{M}} \mathcal{K}_n(\mathcal{P}_{\mathcal{M}}\mathcal{M}^{-1}\mathcal{A}, v) = \text{range}(V_n)$. We decompose the left hand side as

$$\langle [V_n, U], \mathcal{M}^{-1}\mathcal{A}[V_n, U] \rangle_{\mathcal{M}} = \begin{bmatrix} \langle V_n, \mathcal{M}^{-1}\mathcal{A}V_n \rangle_{\mathcal{M}} & \langle V_n, \mathcal{M}^{-1}\mathcal{A}U \rangle_{\mathcal{M}} \\ \langle U, \mathcal{M}^{-1}\mathcal{A}V_n \rangle_{\mathcal{M}} & \langle U, \mathcal{M}^{-1}\mathcal{A}U \rangle_{\mathcal{M}} \end{bmatrix}.$$

The Lanczos relation (2.21) is equivalent to

$$\mathcal{M}^{-1}\mathcal{A}V_n = V_{n+1}\underline{\mathbf{T}}_n + \mathcal{M}^{-1}\mathcal{A}U \langle U, \mathcal{A}U \rangle_H^{-1} \langle \mathcal{A}U, V_n \rangle_H \quad (2.24)$$

from which we can conclude with the $\langle \cdot, \cdot \rangle_{\mathcal{M}}$ -orthonormality of $[V_{n+1}, U]$ that

$$\begin{aligned}\langle V_n, \mathcal{M}^{-1}\mathcal{A}V_n \rangle_{\mathcal{M}} &= \langle V_n, V_{n+1} \rangle_{\mathcal{M}} \underline{\mathbf{T}}_n + \langle V_n, \mathcal{M}^{-1}\mathcal{A}U \rangle_{\mathcal{M}} \langle U, \mathcal{A}U \rangle_H^{-1} \langle \mathcal{A}U, V_n \rangle_H \\ &= \mathbf{T}_n + \langle V_n, \mathcal{A}U \rangle_H \langle U, \mathcal{A}U \rangle_H^{-1} \langle \mathcal{A}U, V_n \rangle_H.\end{aligned}$$

The characterization of Ritz pairs is complete by recognizing that $\mathbf{B} = \langle V_n, \mathcal{M}^{-1}\mathcal{A}U \rangle_{\mathcal{M}} = \langle V_n, \mathcal{A}U \rangle_H = \langle U, \mathcal{M}^{-1}\mathcal{A}V_n \rangle_{\mathcal{M}}^H$ and $\mathbf{E} = \langle U, \mathcal{M}^{-1}\mathcal{A}U \rangle_{\mathcal{M}} = \langle U, \mathcal{A}U \rangle_H$.

Only the residual norm equation remains to show. Therefore we compute with (2.24)

$$\begin{aligned}\mathcal{M}^{-1}\mathcal{A}w - \mu w &= \mathcal{M}^{-1}\mathcal{A}[V_n, U]\tilde{w} - \mu[V_n, U]\tilde{w} \\ &= [V_{n+1}, \mathcal{M}^{-1}\mathcal{A}U, U] \begin{bmatrix} \underline{\mathbf{T}}_n - \mu \underline{\mathbf{I}}_n & 0 \\ \mathbf{E}^{-1}\mathbf{B}^H & \mathbf{I}_k \\ 0 & -\mu \mathbf{I}_k \end{bmatrix} \tilde{w} \\ &= [V_{n+1}, \mathcal{M}^{-1}\mathcal{A}U, U] \mathbf{G} \tilde{w}.\end{aligned}$$

The squared residual $\|\cdot\|_{\mathcal{M}}$ -norm thus is

$$\|\mathcal{M}^{-1}\mathcal{A}w - \mu w\|_{\mathcal{M}}^2 = (\mathbf{G}\tilde{w})^H \langle [V_{n+1}, \mathcal{M}^{-1}\mathcal{A}U, U], [V_{n+1}, \mathcal{M}^{-1}\mathcal{A}U, U] \rangle_{\mathcal{M}} \mathbf{G}\tilde{w}$$

where $\langle [V_{n+1}, \mathcal{M}^{-1}\mathcal{A}U, U], [V_{n+1}, \mathcal{M}^{-1}\mathcal{A}U, U] \rangle_{\mathcal{M}} = \begin{bmatrix} \mathbf{I}_{n+1} & \mathbf{B} & \mathbf{0} \\ \mathbf{B}^H & \mathbf{F} & \mathbf{E} \\ \mathbf{0} & \mathbf{E} & \mathbf{I}_k \end{bmatrix}$ can be shown

with the same techniques as in 1. and 2. \square

REMARK 1. *Lemma 2.7 also holds for the (rare) case that $\mathcal{K}_n(\mathcal{P}_{\mathcal{M}}\mathcal{M}^{-1}\mathcal{A}, v)$ is an invariant subspace of $\mathcal{P}_{\mathcal{M}}\mathcal{M}^{-1}\mathcal{A}$ which we excluded for readability reasons. The Lanczos relation (2.21) in this case is $\mathcal{P}_{\mathcal{M}}\mathcal{M}^{-1}\mathcal{A}V_n = V_n\mathbf{T}_n$ which does not change the result.*

Lemma 2.7 shows how a Lanczos relation for the operator $\mathcal{P}_{\mathcal{M}}\mathcal{M}^{-1}\mathcal{A}$ (that can be generated implicitly in the deflated and preconditioned MINRES algorithm, cf. end of section 2.2) can be used to obtain Ritz pairs of the “undeflated” operator $\mathcal{M}^{-1}\mathcal{A}$. An algorithm for the solution of the sequence of linear systems (2.20) as described in the beginning of this subsection is given in algorithm 1. Additional to the Ritz vectors this algorithm can include auxiliary deflation vectors $Y^{(i)}$.

Algorithm 1 Algorithm for the solution of the sequence of linear systems (2.20).

Input: For $i \in \{1, \dots, M\}$ we have:

- $\mathcal{M}_{(i)} \in L(H)$ is $\langle \cdot, \cdot \rangle_H$ -self-adjoint and positive-definite. \triangleright preconditioner
 - $\mathcal{A}_{(i)} \in L(H)$ is $\langle \cdot, \cdot \rangle_H$ -self-adjoint. \triangleright operator
 - $b^{(i)}, x_0^{(i)} \in H$. \triangleright right hand side and initial guess
 - $Y^{(i)} \in H^{l(i)}$ for $l(i) \in \mathbb{N}_0$. \triangleright auxiliary deflation vectors (may be empty)
- 1: $W = [] \in H^0$ \triangleright no Ritz vectors available in first step
 - 2: **for** $i = 1 \rightarrow M$ **do**
 - 3: $U =$ orthonormal basis of $\text{span}[W, Y^{(i)}]$ with respect to $\langle \cdot, \cdot \rangle_{\mathcal{M}_{(i)}}$.
 - 4: $C = \mathcal{A}_{(i)}U$, $\mathbf{E} = \langle U, C \rangle_H$, set up \mathcal{P}^* \triangleright cf. definition 2.3
 - 5: $x_0 = \mathcal{P}^*x_0^{(i)} + U\mathbf{E}^{-1}\langle U, b^{(i)} \rangle_H$ \triangleright corrected initial guess
 - 6: $x_n^{(i)}, V_{n+1}, \underline{\mathbf{T}}_n, \mathbf{B} = \text{MINRES}(\mathcal{A}_{(i)}, b^{(i)}, \mathcal{M}_{(i)}^{-1}, \mathcal{P}^*, x_0, \varepsilon)$
 - | MINRES is applied to $\mathcal{M}_{(i)}^{-1}\mathcal{A}_{(i)}x^{(i)} = \mathcal{M}_{(i)}^{-1}b^{(i)}$ with inner product $\langle \cdot, \cdot \rangle_{\mathcal{M}_{(i)}}$, right preconditioner \mathcal{P}^* , initial guess x_0 and tolerance $\varepsilon > 0$, cf. section 2.2. Then:
 - The approximation $x_n^{(i)}$ fulfills $\left\| \mathcal{M}_{(i)}^{-1}b^{(i)} - \mathcal{M}_{(i)}^{-1}\mathcal{A}_{(i)}x_n^{(i)} \right\|_{\mathcal{M}_{(i)}} \leq \varepsilon$.
 - The Lanczos relation $\mathcal{M}_{(i)}^{-1}\mathcal{A}_{(i)}\mathcal{P}^*V_n = V_{n+1}\underline{\mathbf{T}}_n$ holds.
 - $\mathbf{B} = \langle V_n, C \rangle_H$ is generated as a byproduct of the application of \mathcal{P}^* .
 - 7: $w_1, \dots, w_m, \mu_1, \dots, \mu_m, \rho_1, \dots, \rho_m = \text{Ritz}(U, V_{n+1}, \underline{\mathbf{T}}_n, \mathbf{B}, C, \mathbf{E}, \mathcal{M}_{(i)}^{-1})$
 - | Ritz(...) computes the Ritz pairs (w_j, μ_j) for $j \in \{1, \dots, m\}$ of $\mathcal{M}_{(i)}^{-1}\mathcal{A}_{(i)}$ with respect to $\text{span}[U, V_n]$ and the inner product $\langle \cdot, \cdot \rangle_{\mathcal{M}_{(i)}}$, cf. lemma 2.7.
 - | Then:
 - w_1, \dots, w_m form a $\langle \cdot, \cdot \rangle_{\mathcal{M}_{(i)}}$ -orthonormal basis of $\text{span}[U, V_n]$.
 - The residual norms $\rho_j = \left\| \mathcal{M}_{(i)}^{-1}\mathcal{A}_{(i)}w_j - \mu_j w_j \right\|_{\mathcal{M}_{(i)}}$ are also returned.
 - 8: $W = [w_{i_1}, \dots, w_{i_k}]$ for pairwise distinct $i_1, \dots, i_k \in \{1, \dots, m\}$.
 - | Pick k Ritz vectors according to Ritz value and residual norm.
 - 9: **end for**
-

	Applications of			Inner products	Vector updates
	\mathcal{A}	\mathcal{M}^{-1}	\mathcal{M}		
Orthogonalization	–	–	k	$k(k+1)/2$	$k(k+1)/2$
Setup of \mathcal{P}^* and initial guess x_0	k	–	–	$k(k+5)/2$	$2k$
n MINRES iterations	n	n	–	$n(k+2)$	$n(k+7)$
Computation of Ritz vectors	–	k	–	k^2	$k(k+n)$

Table 2.2: Computational cost for one iteration of algorithm 1 (lines 3–8) with n MINRES iterations and k deflation vectors. The number of computed Ritz vectors also is k . Operations that do not depend on the dimension $N := \dim H$ are neglected.

Implementational notes. We now comment on the implementational side of the determination and utilization of Ritz pairs while solving a sequence of linear systems (cf. algorithm 1). The solution of a single linear system with the deflated and preconditioned MINRES method was discussed in section 2.2. Although the MINRES method is based on short recurrences due to the underlying Lanczos algorithm – and thus only needs storage for a few vectors – we still have to store the full Lanczos basis V_{n+1} for the determination of Ritz vectors. The Lanczos matrix $\underline{\mathbf{T}}_n \in \mathbb{R}^{n+1,n}$ is no issue because it is tridiagonal and symmetric. However, by employing a “good” preconditioner that limits the number of iterations we are able to satisfy memory constraints in many applications (cf. section 3.3). Deflation can then be used to further improve convergence by directly addressing parts of the preconditioned operator’s spectrum. An annotated version of the algorithm can be found in algorithm 1. Note that the orthonormalization in line 3 is redundant in exact arithmetic if only Ritz vectors are used and the preconditioner does not change. An overview of the computational cost of one iteration of algorithm 1 is given in table 2.2.

3. Application to nonlinear Schrödinger problems. Given an open domain $\Omega \subseteq \mathbb{R}^d$, $d \in \{2, 3\}$, nonlinear Schrödinger operators are typically derived from the minimization of the Gibbs energy in a corresponding physical system and have the form

$$\begin{aligned} \mathcal{S}(\psi) &: X \rightarrow Y, \\ \mathcal{S}(\psi) &:= (\mathcal{K} + V + g|\psi|^2)\psi \quad \text{in } \Omega \end{aligned} \tag{3.1}$$

with $X \subseteq L^2(\Omega)$ being the natural energy space of the problem, Y its dual. If the domain is bounded, the energy space X may incorporate boundary conditions appropriate to the physical setting. The linear operator \mathcal{K} is assumed to be symmetric and positive-semidefinite, $V : \Omega \rightarrow \mathbb{R}$ be a given scalar potential, and $g \in \mathbb{R}$ a given coupling parameter. A state $\hat{\psi} : \Omega \rightarrow \mathbb{C}$ is called a solution of the nonlinear Schrödinger equation if

$$\mathcal{S}(\hat{\psi}) = 0. \tag{3.2}$$

Generally, one is only interested in nontrivial solutions $\hat{\psi} \neq 0$. The function $\hat{\psi}$ is often referred to as *order parameter* and its magnitude $|\hat{\psi}|^2$ typically describes a particle density or, more general, a probability distribution. Note that, because of

$$\mathcal{S}(\exp\{i\chi\}\psi) = \exp\{i\chi\}\mathcal{S}(\psi) \tag{3.3}$$

one solution $\hat{\psi} \in X$ is really just a representative of the physically equivalent solutions $\{\exp\{i\chi\}\hat{\psi} : \chi \in \mathbb{R}\}$.

For the numerical solution of (3.2), Newton's method is the method of choice. Given a good-enough initial guess ψ_0 , the Newton process generates a sequence of iterates ψ_k which converges towards a solution $\hat{\psi}$ of (3.2). In each step k of Newton's method, a linear system with the Jacobian $\mathcal{J}(\psi_k)$ of \mathcal{S} at ψ_k needs to be solved. The linear operator $\mathcal{J}(\psi)$ is given by

$$\begin{aligned} \mathcal{J}(\psi) : X &\rightarrow Y, \\ \mathcal{J}(\psi)\varphi &:= (\mathcal{K} + V + 2g|\psi|^2)\varphi + g\psi^2\bar{\varphi}. \end{aligned} \quad (3.4)$$

Despite the fact that states ψ are generally complex-valued, $\mathcal{J}(\psi)$ is linear only if X and Y are defined as vector spaces over the field \mathbb{R} with the corresponding inner product

$$\langle \cdot, \cdot \rangle_{\mathbb{R}} := \Re \langle \cdot, \cdot \rangle_{L^2(\Omega)}. \quad (3.5)$$

This matches the notion that the specific complex argument of the order parameter is of no physical relevancy since $|\alpha\psi|^2 = ||\alpha|\psi|^2$ for all $\alpha \in \mathbb{C}$, $\psi \in X$ (compare with (3.3)).

Moreover, the work in [28] gives a representation of adjoints of operators of the form (3.4), from which one can derive

COROLLARY 1. *For any given $\psi \in Y$, the Jacobian operator $\mathcal{J}(\psi)$ (3.4) is self-adjoint with respect to the inner product (3.5).*

An important consequence of the independence of states of the complex argument (3.3) is the fact that solutions of (3.10) form a smooth manifold in X . This results in the linearization (3.4) in solutions always having a nontrivial kernel. Indeed, for any $\psi \in X$

$$\mathcal{J}(\psi)(i\psi) = (\mathcal{K} + V + 2g|\psi|^2)(i\psi) - gi\psi^2\bar{\psi} = i(\mathcal{K} + V + g|\psi|^2)\psi = i\mathcal{S}(\psi), \quad (3.6)$$

so for nontrivial solutions $\hat{\psi} \in X$, $\psi \neq 0$, $F(\hat{\psi}) = 0$, the dimension of the kernel of $\mathcal{J}(\psi)$ is at least 1.

Besides the fact that there is always a zero eigenvalue in a solution ψ_s and that all eigenvalues are real, not much more can be said about the spectrum; in general, $\mathcal{J}(\psi)$ is indefinite. The definiteness depends entirely on the state ψ ; if ψ is a solution to (3.1), it is said to be stable or unstable depending whether or not $\mathcal{J}(\psi)$ has negative eigenvalues. Typically, solutions with low energies tend to be stable whereas highly energetic solutions tend to be unstable. For physical systems in practice, it is uncommon to see more than ten negative eigenvalues for a given solution state.

3.1. Principal problems for the numerical solution. While the numerical solution of nonlinear systems itself is challenging, the presence of a singularity in a solution as in (3.6) adds two major obstacles for using Newton's method.

- Newton's method is guaranteed to converge towards a solution \hat{x} Q -superlinearly in the area of attraction only if \hat{x} is nondegenerate, i.e., the Jacobian in \hat{x} is regular. If the Jacobian operator does have a singularity, only linear convergence can be guaranteed.
- While no linear system has to be solved with the exactly singular $\mathcal{J}(\hat{\psi})$, the Jacobian operator close the solution $\mathcal{J}(\hat{\psi} + \delta\psi)$ will have at least one eigenvalue of small magnitude, i.e., the Jacobian system becomes ill-conditioned when approaching a solution.

Several approaches have been suggested to deal with this situation, for a concise survey of the matter, see [13]. One of the most used strategies is *bordering* which suggests extending the original problem $\mathcal{S}(\psi) = 0$ by a so-called *phase condition* to pin down the redundancy [1],

$$0 = \tilde{\mathcal{S}}(\psi, \lambda) := \begin{pmatrix} \mathcal{S}(\psi) + \lambda y \\ p(x) \end{pmatrix}. \quad (3.7)$$

If y and $p(\cdot)$ are chosen according to some well-understood criteria [14], the Jacobian systems can be shown to be well-conditioned throughout the Newton process. Moreover, the bordering can be chosen in such a way that the linearization of the extended system is self-adjoint in extended scalar product if the linearization of the original problem was self-adjoint. This method has been applied to the specialization of the Ginzburg–Landau equations before [28] (3.10), and naturally generalizes to nonlinear Schrödinger equations in the same way. The major disadvantage of the bordering approach, however, is that it is not clear how to precondition the extended system even if a good preconditioner for the original problem is known. This renders bordering unfeasible for the discretization of nonlinear PDEs with a large number of unknowns.

In the particular case of nonlinear Schrödinger equations, the loss of speed of convergence is less severe than in more general settings. Note that there would be no slowdown at all if the Newton update $\delta\psi$, given by

$$\mathcal{J}(\psi)\delta\psi = -\mathcal{S}(\psi), \quad (3.8)$$

was consistently orthogonal to the null space $i\hat{\psi}$ close to a solution $\hat{\psi}$. While this is not generally true, one is at least in the situation that the Newton update can never be an exact multiple of the direction of the approximate null space $i\psi$. This is because

$$\mathcal{J}(\psi)(\alpha i\psi) = -\mathcal{S}(\psi), \quad \alpha \in \mathbb{R},$$

together with (3.6), is equivalent to

$$\alpha i\mathcal{S}(\psi) = -\mathcal{S}(\psi)$$

which can only be fulfilled if $\mathcal{S}(\psi) = 0$, i.e., if ψ is already a solution.

Consequently, loss of Q -superlinear convergence is hardly ever observed in numerical experiments. Figure 3.1, for example, shows the Newton residual for the two- and three-dimensional test setups, both with the standard formulation and with the bordering 3.7 as proposed in [28]. Of course, the Newton iterates follow different trajectories, but the important thing to note is that in both plain and bordered formulation, the speed of convergence close the solution is comparable.

The more severe restriction is in the numerical difficulty of solving the Jacobian systems in each Newton step due to the increasing ill-posedness of the problem as described above. However, although the Jacobian has a nontrivial near-null space close to a solution, the problem is well-defined at all times. This is because, by self-adjointness, its left near-null space coincides with the right near-null space, $\text{span}\{i\hat{\psi}\}$, and the right-hand-side in (3.8), $-\mathcal{S}(\psi)$, is orthogonal to $i\psi$ for any ψ :

$$\begin{aligned} \langle i\psi, \mathcal{S}(\psi) \rangle_{\mathbb{R}} &= \langle i\psi, \mathcal{K}(\psi) \rangle_{\mathbb{R}} + \langle i\psi, V(\psi) \rangle_{\mathbb{R}} + \langle i\psi, g|\psi|^2\psi \rangle_{\mathbb{R}} \\ &= \Re \langle i\psi, \mathcal{K}\psi \rangle_2 + \Re \langle i\psi, V\psi \rangle_2 + \Re (gi \langle |\psi|^2, |\psi|^2 \rangle_2) = 0. \end{aligned} \quad (3.9)$$

The numerical problem is hence caused only by the fact that one eigenvalue approaches the origin as the Newton iterates approach a solution. The authors propose to handle this difficulty on the level of the linear solves for the Newton updates using the deflation framework developed in section 2.

3.2. The Ginzburg–Landau equation. One important instance of nonlinear Schrödinger equations (3.1) is the Ginzburg–Landau equation that models supercurrent density for extreme-type-II superconductors. Given an open, bounded domain $\Omega \subseteq \mathbb{R}^d$, $d \in \{2, 3\}$, the equations are

$$0 \stackrel{!}{=} \begin{cases} \mathcal{K}\psi - \psi(1 - |\psi|^2), \\ \mathbf{n} \cdot (-i\nabla - \mathbf{A})\psi. \end{cases} \quad (3.10)$$

The operator \mathcal{K} is defined as

$$\begin{aligned} \mathcal{K}: X &\rightarrow Y, \\ \mathcal{K}\varphi &:= (-i\nabla - \mathbf{A})^2\varphi. \end{aligned} \quad (3.11)$$

with the magnetic vector potential $\mathbf{A} \in H_{\mathbb{R}^d}^2(\Omega)$ [5]. The operator \mathcal{K} describes the energy of a charged particle under the influence of a magnetic field $\mathbf{B} = \nabla \times \mathbf{A}$, and can be shown to be Hermitian and positive-semidefinite; the eigenvalue 0 is assumed only for $\mathbf{A} \equiv \mathbf{0}$ [29]. Solutions $\hat{\psi}$ of (3.10) describe the density $|\hat{\psi}|^2$ of electric charge carriers and fulfill $0 \leq |\hat{\psi}|^2 \leq 1$ pointwise [16]. For two-dimensional domains, they typically exhibit isolated zeros referred to as *vortices*; in three dimensions, lines of zeros are the typical solution pattern (see figure 3.2).

Discretization. For the numerical experiments in this paper, a finite-volume-type discretization is employed [4, 29]. Let $\Omega^{(h)}$ be a discretization of Ω with a triangulation $\{T_i\}_{i=1}^m$, $\bigcup_{i=1}^m T_i = \Omega^{(h)}$, and the node-centered Voronoi tessellation $\{V_k\}_{k=1}^n$, $\bigcup_{k=1}^n V_k = \Omega^{(h)}$. Let further $e_{i,j}$ denote the edge between two nodes i, j . The discretized problem is then to find $\psi^{(h)} \in \mathbb{C}^n$ such that

$$\forall k \in \{1, \dots, n\}: \quad 0 = \left(S^{(h)}\psi^{(h)}\right)_k := \left(K^{(h)}\psi^{(h)}\right)_k - \psi_k^{(h)} \left(1 - |\psi_k^{(h)}|^2\right), \quad (3.12)$$

where the discrete kinetic energy operator $K^{(h)}$ is defined by

$$\begin{aligned} \forall \phi^{(h)}, \psi^{(h)} \in \mathbb{C}^n: \quad \left\langle K^{(h)}\psi^{(h)}, \phi^{(h)} \right\rangle = \\ \sum_{\text{edges } e_{i,j}} \alpha_{i,j} \left[\left(\psi_i^{(h)} - U_{i,j}\psi_j^{(h)}\right) \overline{\phi_i^{(h)}} + \left(\psi_j^{(h)} - \overline{U_{i,j}}\psi_i^{(h)}\right) \overline{\phi_j^{(h)}} \right] \end{aligned} \quad (3.13)$$

with the discrete inner product

$$\left\langle \psi^{(h)}, \phi^{(h)} \right\rangle := \sum_{k=1}^n |V_k| \psi_k^{(h)} \overline{\phi_k^{(h)}}$$

and edge coefficients $\alpha_{i,j} \in \mathbb{R}$ [29]. The magnetic vector potential \mathbf{A} is incorporated in the so-called *link variables*,

$$U_{i,j} := \exp \left(-i \int_{\mathbf{x}_j}^{\mathbf{x}_i} \mathbf{e}_{i,j} \cdot \mathbf{A}(\mathbf{w}) \, d\mathbf{w} \right).$$

along the edges $e_{i,j}$ of the triangulation.

REMARK 2. *In matrix form, the operator $K^{(h)}$ is represented as a product $K^{(h)} = D^{-1}\widehat{K}$ of the diagonal matrix D^{-1} , $D_{i,i} = |V_i|$, and a Hermitian matrix \widehat{K} .*

This discretization preserves a number of invariants of the problem, e.g., gauge invariance of the type $\tilde{\psi} := \exp\{i\chi\}$, $\tilde{\mathbf{A}} := \mathbf{A} + \nabla\chi$ with a given $\chi \in C^1(\Omega)$. Moreover, the discretized energy operator $K^{(h)}$ is Hermitian and positive-definite [29]. The discretized Jacobian operator is self-adjoint with respect to the discrete inner product

$$\left\langle \psi^{(h)}, \phi^{(h)} \right\rangle_{\mathbb{R}} := \Re \left(\sum_{k=1}^n |V_k| \overline{\psi_k^{(h)}} \phi_k^{(h)} \right) \quad (3.14)$$

and the statements (3.6), (3.9) about the null space carry over from the continuous formulation.

REMARK 3 (Real-valued formulation). *There is a vector space isomorphism $\alpha : \mathbb{C}^n \rightarrow \mathbb{R}^{2n}$ between \mathbb{R}^{2n} and \mathbb{C}^n as vector space over \mathbb{R} given by the basis mapping*

$$\alpha(e_j^{(n)}) = e_j^{(2n)}, \quad \alpha(i e_j^{(n)}) = e_{n+j}^{(2n)}.$$

In particular, note that the dimension of $\mathbb{C}_{\mathbb{R}}^n$ is $2n$. The isomorphism α is also isometric with the natural inner product $\langle \cdot, \cdot \rangle_{\mathbb{R}}$ of $\mathbb{C}_{\mathbb{R}}^n$, since for any given pair $\phi, \psi \in \mathbb{C}^n$ one has

$$\left\langle \begin{pmatrix} \Re\phi \\ \Im\phi \end{pmatrix}, \begin{pmatrix} \Re\psi \\ \Im\psi \end{pmatrix} \right\rangle = \langle \Re\phi, \Re\psi \rangle + \langle \Im\phi, \Im\psi \rangle = \langle \phi, \psi \rangle_{\mathbb{R}}.$$

Moreover, linear operators over $\mathbb{C}_{\mathbb{R}}^n$ generally have the form $L\psi = A\psi + B\overline{\psi}$ with some $A, B \in \mathbb{C}^{n \times n}$ and because of

$$Lw = \lambda w \quad \Leftrightarrow \quad (\alpha L \alpha^{-1})\alpha w = \lambda \alpha w,$$

the spectral properties also exactly convey to its real-valued image $\alpha L \alpha^{-1}$.

This equivalence can be relevant in practice as quite commonly, the original complex-valued problem in \mathbb{C}^n is implemented in terms \mathbb{R}^{2n} . Using the natural inner product in this space will yield the expected results without having to take particular care of the inner product.

3.3. Numerical experiments. The numerical experiments are performed with the following two setups.

TEST SETUP 1 (2D). *The circle $\Omega_{2D} := \{x \in \mathbb{R}^2 : \|x\|_2 < 5\}$ and the magnetic vector potential $\mathbf{A}(x) := \mathbf{m} \times (x - x_0) / \|x - x_0\|^3$ with $\mathbf{m} := (0, 0, 1)^T$ and $x_0 := (0, 0, 5)^T$, corresponding to the magnetic field generated by a dipole at x_0 with orientation \mathbf{m} . A Delaunay triangulation for this domain was created using Triangle [30], bearing 3299 points. With the discrete equivalent of $\psi_0(x) = \cos(\pi x)$ as initial guess, the Newton process converges after 27 iterations with a residual of less than 10^{-10} in the discretized norm (see figure 3.1). The final state is illustrated in figure 3.2.*

TEST SETUP 2 (3D). *The three-dimensional L-shape*

$$\Omega_{3D} := \{x \in \mathbb{R}^3 : \|x\|_{\infty} < 5\} \setminus \mathbb{R}_+^3,$$

discretized using Gmsh [11] with 72166 points. The chosen magnetic vector field is constant $\mathbf{B}_{3D}(x) := 3^{-1/2}(1, 1, 1)^T$, represented by the vector potential $\mathbf{A}_{3D}(x) :=$

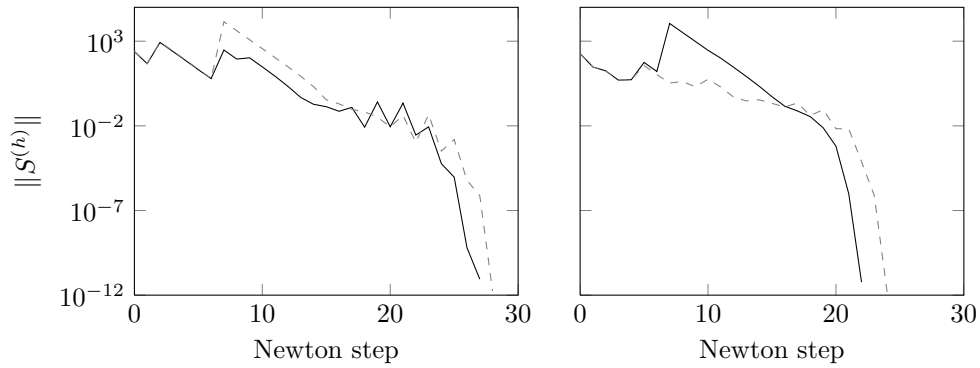


Fig. 3.1: Newton residual history for the two-dimensional setup 1 (left) and three-dimensional setup 2 (right), each with bordering (---) and without (—). With initial guesses $\psi_0^{2D}(\mathbf{x}) = \cos(\pi y)$ and $\psi_0^{3D}(\mathbf{x}) = 1$, respectively, the Newton process delivered the solutions as highlighted in figure 3.2 in 22 and 27 steps, respectively.

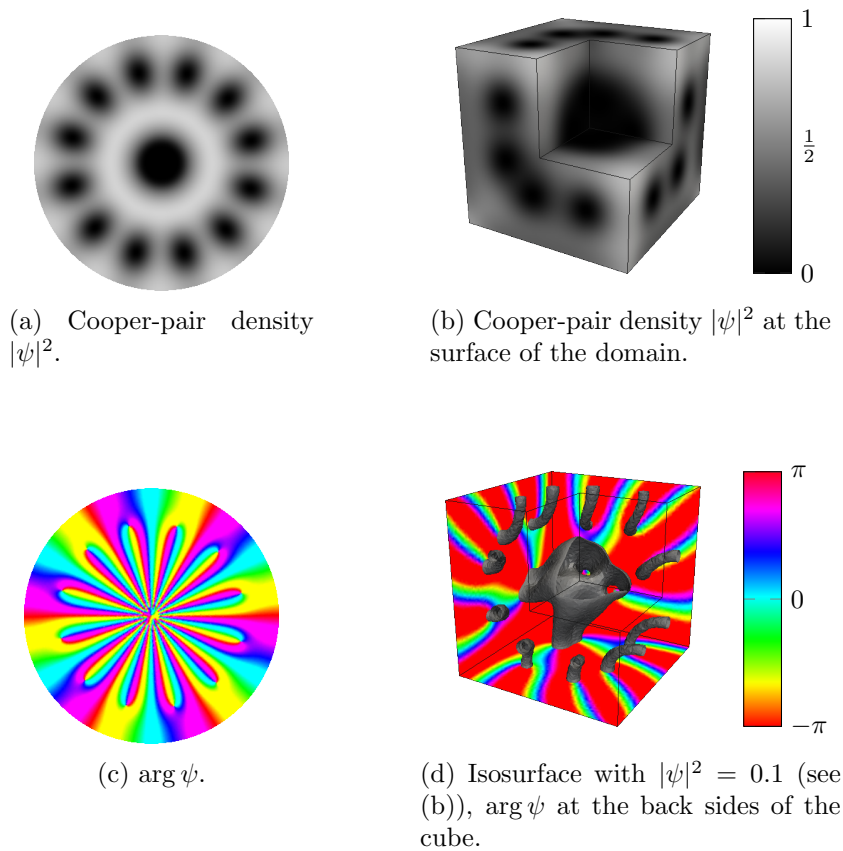


Fig. 3.2: Solutions of the test problems as found in the Newton process illustrated in figure 3.1.

$\frac{1}{2}\mathbf{B}_{3D} \times \mathbf{x}$. With the discrete equivalent of $\psi_0(\mathbf{x}) = 1$, the Newton process converges after 22 iterations with a residual of less than 10^{-10} in the discretized norm (see figure 3.1). The final state is illustrated in figure 3.2.

For both of representative setups, a Newton run was performed where the linear systems (3.8) were solved using MINRES to exploit self-adjointness of $J^{(h)}$. Note that it is critical here to use the natural inner product of the system, (3.14). All of the numerical experiments incorporate the preconditioner proposed in [29] that is shown to bound the number of Krylov iterations needed to reach a certain relative residual by a constant independently of the number n of unknowns in the system.

REMARK 4. *Neither of the above test problems have initial guesses which sit in the cone of attraction of the solution they eventually converge to. As typical for local nonlinear solvers, the iterations which do not directly correspond with the final convergence are sensitive to effects introduced by the discretization or round-off errors. It will hence be difficult to reproduce the shown solutions without exact information about the point coordinates in the discretization mesh. Nevertheless, the numerical results hold true for any converging Newton iteration, independently of their final state.*

Figure 3.3 shows the relative residuals for all Newton steps in both the two- and the three-dimensional setup. Note that the residual curves late in the Newton process (dark gray) exhibit plateaus of stagnation which are attributed to the low-magnitude eigenvalue associated with the near-null space vector $i\psi^{(h)}$.

Figure 3.3b incorporates deflation of said vector via the framework as described in section 2. The incorporation of the preconditioner and the customized inner product 3.14 is crucial here. Clearly, the stagnation effects are remedied and a significantly lower number of iterations is necessary to reduce the residual norm to 10^{-10} . While this comes with extra computational cost per step (cf. table 2.1), this cost is negligible compared to the considerable convergence speedup.

REMARK 5. *Note that the initial guess \tilde{x}_0 is adapted according to (2.16) before the beginning the iteration. Because of that, the initial relative residual $\|b - Ax_0\|/\|b - A\tilde{x}_0\|$ cannot generally be expected to equal 1 even if $\tilde{x}_0 = 0$. In the particular case of $U = i\psi$, however, we have*

$$x_0 = \mathcal{P}^* \tilde{x}_0 + U \langle U, J(\psi)U \rangle_{\mathbb{R}}^{-1} \langle U, -\mathcal{S}(\psi) \rangle_{\mathbb{R}} = \mathcal{P}^* \tilde{x}_0$$

since $\langle i\psi, \mathcal{S}(\psi) \rangle = 0$ (3.9), and the initial relative residual does equal 1 if $\tilde{x}_0 = 0$ (cf. figure 3.3b). Note that this is not true anymore when more deflation vectors are added (cf. figure 3.3c).

As indicated in section 2, the idea of deflation can be taken further by noting that, towards the end of the Newton process, a series of very similar linear systems needs to be solved. This leads to the idea of extracting spectral information of the previous MINRES iteration use for deflation in the present process. For the experiments, those 12 Ritz vectors from the MINRES iteration in Newton step k which belong to the Ritz values of smallest magnitude were added for deflation in Newton step $k+1$. As displayed in figure 3.3c, the number of necessary Krylov iterations is further decreased roughly by a factor of 2. Note also that in particular, the characteristic plateaus corresponding with the low-magnitude eigenvalue to not anymore occur. This is particularly interesting since no information about the approximate null space was explicit specified, but automatically extracted from previous Newton steps.

Technically, one could go ahead and extract even more Ritz vectors for deflation in the next step. However, at some point the extra cost associated with the extraction of

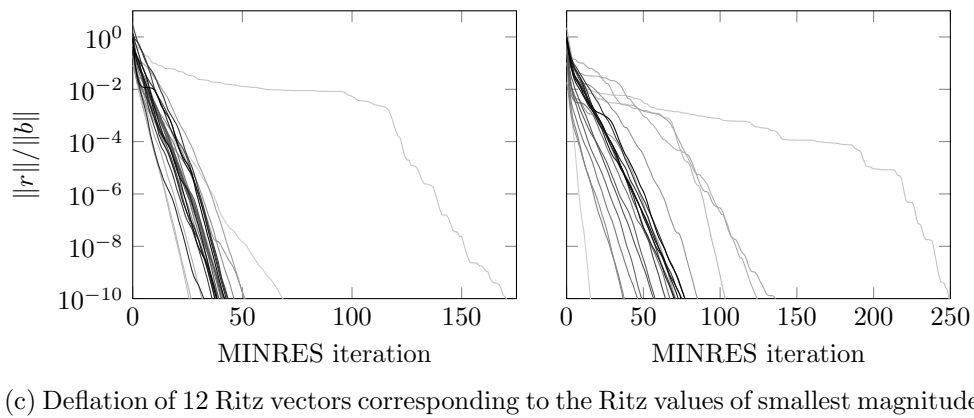
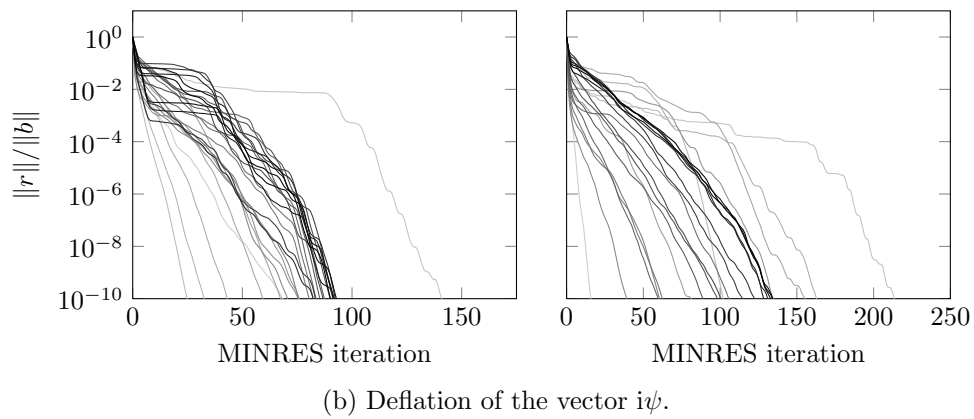
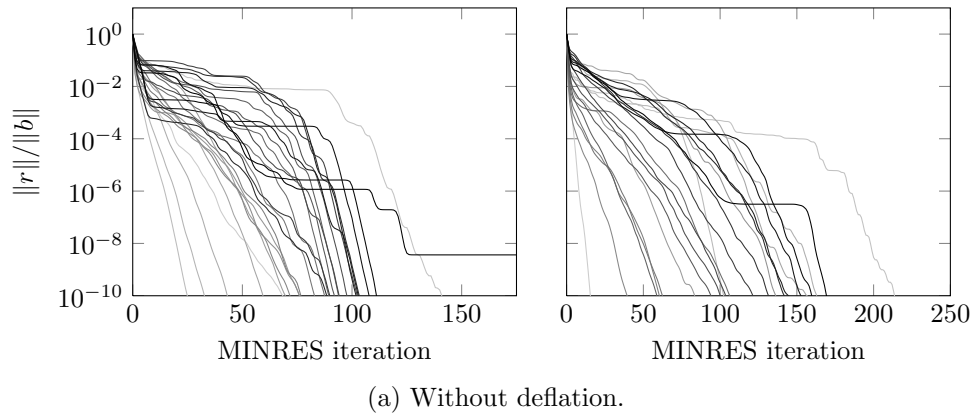


Fig. 3.3: MINRES convergence histories of all Newton steps for the 2D problem (left) and 3D problem (right). The color of the curve corresponds to the Newton step: light gray is the first Newton step while black is the last Newton step.

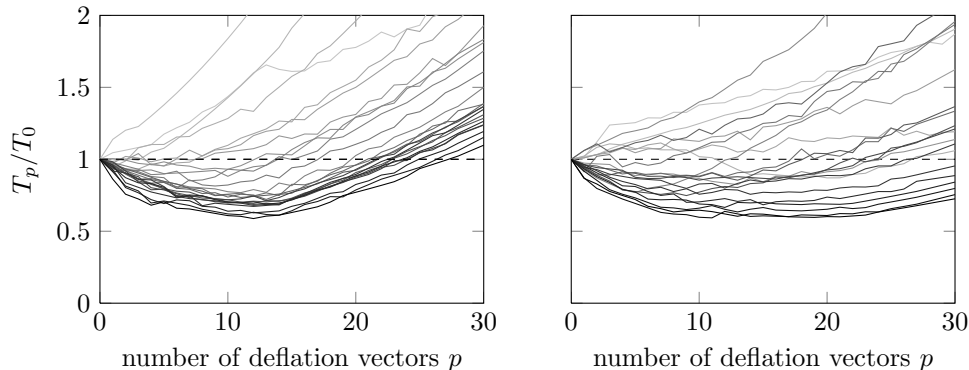


Fig. 3.4: Wall-times T_p needed for MINRES solves for the test setups with deflation of those p Ritz vectors from the previous Newton step which correspond to the smallest Ritz values. As in the figure 3.3, light gray lines correspond to steps early in the Newton process. All times are displayed relative to the computing time T_0 without deflation. The dashed line at $T_p/T_0 = 1$ marks the threshold below which deflation pays off.

the Ritz vectors (table 2.2) and the application of the projection operator (table 2.1) will not justify a further increase of the deflation space. The efficiency threshold will be highly dependent on the cost of the preconditioner. Moreover, it is in most situations impossible to predict just how the deflation of a particular set of vectors influences the residual behavior in a Krylov process. For this reason, one has to reside to numerical experiments to estimate the optimal dimension of the deflation space. Figure 3.4 shows, again for all Newton steps in both setups, the wall time of the Krylov iterations as in figure 3.3 relative to the solution time without deflation. The experiments show that deflation in the first few Newton steps does not accelerate the computing speed. This is due to the fact that the Newton updates are still significantly large and the subsequent linear systems are too different from each other to take profit from carrying over spectral information. As the Newton process advances and the updates become smaller, the subsequent linear systems become similar and deflation of a number of vectors becomes profitable. Note, however, that there is a point at which the computational cost of extraction and application of the projection exceeds the gain in Krylov iterations. For the two-dimensional setup, this value is around 12 while in the three-dimensional case, the minimum roughly stretches from 10 to 20 deflated Ritz vectors. In both cases, a reduction of effective computation time by 40% could be achieved.

REMARK 6. *Note that throughout the numerical experiments performed in this paper, the linear systems were solved in up to the relative residual of 10^{-10} . In practice, however, one would employ a relaxation scheme as given in, e.g., [6, 25]. Those schemes commonly advocate a relaxed relative tolerance η_k in regions of slow convergence, and a more stringent condition when the speed of convergence accelerates toward a solution, e.g.,*

$$\eta_k = \gamma \left(\frac{\|F_k\|}{\|F_{k-1}\|} \right)^\alpha$$

with some $\gamma > 0$, $\alpha > 1$. In the specific case of nonlinear Schrödinger equations, this means that deflation of the near-null vector $i\psi$ (cf. figure 3.3b) becomes little effective if η_k is higher than where the stagnation plateau appears. The speedup associated with deflation with a number of Ritz vectors (cf. figure 3.3c), however, is effective throughout the Krylov iteration and would hence not be influenced by a premature abortion of the process.

REMARK 7. As opposed to the CG method, there is no consensus on what implementation of the MINRES procedure is least prone to round-off errors. In general, the MINRES iteration can be unstable to the point of complete stagnation well above machine precision [33] (see the stagnating process in figure 3.3a). This is attributed to the implicit loss of orthogonality of the Ritz vectors due to round-off errors and can thus be remedied by storing all computed Ritz vectors and reorthogonalizing against the set in each MINRES iteration. This essentially leads to the GMRES process.

All numerical experiments in this paper have been conducted with and without explicit reorthogonalization and despite the observation of a loss of orthogonality in the Ritz vectors, the convergence speedup with Ritz vectors from the previous step was not noticeably affected.

REMARK 8. The methods described and developed in this paper are implemented in the Python package `pynosh` [9] made available under a free and open source license (GNU General Public License 3). All experimental results presented in this section can be reproduced from the data published with the source code.

4. Conclusions. For the solution of a sequence of self-adjoint linear systems such as occurring in Newton process for a large class of nonlinear problems, the authors propose a MINRES scheme that takes into account spectral information from the previous linear systems. Central to the approach is the cheap extraction of Ritz vectors (section 2.3) out of a MINRES iteration and the application of the projection (2.10). As opposed to similar recycling methods previously suggested [36], the present one consistently preserved self-adjointness of the projected operator, explicitly incorporates the use of a preconditioner, and allows for inner products other than the default ℓ_2 -inner product.

These properties are then crucial for the application to nonlinear Schrödinger equations (section 3): The occurring linearization is self-adjoint with respect to a nonstandard inner product (3.14), and the computation in a three-dimensional setting is not feasible without a preconditioner. The authors could show that for the particular case of the Ginzburg–Landau equations, the deflation strategy reduces the effective run time of a linear solve by up to 40% (cf. figure 3.3c). Moreover, the deflation strategy was shown to automatically handle the singularity of the problem that otherwise leads to numerical instabilities.

It is expected that the strategy will perform similarly for other nonlinear problems. While adding a number of vectors to the deflation will always lead to faster Krylov convergence, it only comes with extra computational cost in extracting the Ritz vector and applying the projection operator. The optimal number of deflated Ritz vectors is highly problem-dependent, in particular the computational cost of the preconditioner, and can thus hardly be determined a priori.

The proposed strategy naturally extends to problems which are not self-adjoint by choosing, e.g., GMRES as the hosting Krylov method. For asymmetric problems, however, the effects of altered spectra on the Krylov convergence is far more involved than in the self-adjoint case [20]. This also makes the choice of Ritz vectors for deflation difficult.

Acknowledgments. The authors wish to thank Jörg Liesen for his valuable feedback.

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