

RIEMANNIAN OPTIMISATION METHODS FOR GROUND STATES OF MULTICOMPONENT BOSE–EINSTEIN CONDENSATES

ROBERT ALTMANN, MARTIN HERMANN, DANIEL PETERSEIM, AND TATJANA STYKEL

ABSTRACT. This paper addresses the computation of ground states of multicomponent Bose–Einstein condensates, defined as the global minimiser of an energy functional on an infinite-dimensional generalised oblique manifold. We establish the existence of the ground state, prove its uniqueness up to scaling, and characterise it as the solution to a coupled nonlinear eigenvector problem. By equipping the manifold with several Riemannian metrics, we introduce a suite of Riemannian gradient descent and Riemannian Newton methods. Metrics that incorporate first- or second-order information about the energy are particularly advantageous, effectively preconditioning the resulting methods. For a Riemannian gradient descent method with an energy-adaptive metric, we provide a qualitative global and quantitative local convergence analysis, confirming its reliability and robustness with respect to the choice of the spatial discretisation. Numerical experiments highlight the computational efficiency of both the Riemannian gradient descent and Newton methods.

Key words. Multicomponent Bose–Einstein condensates, coupled Gross–Pitaevskii eigenvalue problem, nonlinear eigenvector problem, Riemannian optimisation, energy-adaptive methods

AMS subject classifications. 66N25, 81Q10, 35Q55

1. INTRODUCTION

This paper is devoted to the numerical approximation of ground states of multicomponent Bose–Einstein condensates (BECs), where p different species of matter can condense into one single internal state with p components; see [13, 25, 26] for an introduction. For the special case of two species and two components, we refer to [14, 49] and [15, Sect. 9.2]. Multicomponent systems can also be obtained, under some simplifying assumptions, from spinor BECs which provide a valuable tool for exploring complex quantum phenomena [16, 18].

Mathematically, a stationary quantum state of a p -component condensate can be modelled as a wave function $\varphi = (\varphi_1, \dots, \varphi_p)$, defined in a domain $\Omega \subset \mathbb{R}^d$, $d = 1, 2, 3$. The components of the wave function φ are square integrable with square integrable weak derivatives. Their squared L^2 -norms represent the masses of the components which are subject to the constraints

$$(1.1) \quad \|\varphi_j\|_{L^2(\Omega)}^2 = N_j > 0, \quad j = 1, \dots, p,$$

where N_j is the given number of particles in the j -th condensate component, and $N_1 + \dots + N_p$ is the total number of particles of the condensate. The set of admissible quantum states of the condensates thus forms an infinite-dimensional generalised oblique manifold. Given the finite mass, the wave function is well approximated in a sufficiently large but bounded domain Ω with homogeneous Dirichlet boundary conditions. Furthermore, the linear combinations $\rho_1(\varphi), \dots, \rho_p(\varphi)$ of the density functions $|\varphi_i|^2$ are given by

$$\rho_j(\varphi) = \sum_{i=1}^p \kappa_{ij} |\varphi_i|^2, \quad j = 1, \dots, p,$$

where the parameters $\kappa_{ij} \in \mathbb{R}$, $\kappa_{ij} = \kappa_{ji}$, characterise the strength of particle interactions between the i -th and j -th condensate components. These interactions can be either attractive ($\kappa_{ij} < 0$) or repulsive ($\kappa_{ij} > 0$).

The energy of the condensate is given by the functional

$$(1.2) \quad \mathcal{E}(\varphi) = \sum_{j=1}^p \int_{\Omega} \frac{1}{2} \|\nabla \varphi_j\|^2 + \frac{1}{2} V_j(x) |\varphi_j|^2 + \frac{1}{4} \rho_j(\varphi) |\varphi_j|^2 dx,$$

M. Hermann and D. Peterseim acknowledge the support of the European Research Council through the project 865751 – RandomMultiScales.

where V_1, \dots, V_p denote the external potentials, which can be, for example, harmonic traps or periodic potentials created by optical lattices or realisations of random potentials created by laser speckles. The first term in (1.2) represents the kinetic energy of the j -th component, the second term is the potential energy, and the last term characterises the energy resulting from particle interactions. The coupling is encoded in the nonlinearities ρ_j and driven by the parameters κ_{ij} , whose relative variation can significantly impact the ground state. In the two-component case $p = 2$, for example, the parameter

$$\Delta_{\text{misc}} = \frac{\kappa_{11}\kappa_{22}}{\kappa_{12}^2} - 1$$

describes the miscibility of the condensate. For $\Delta_{\text{misc}} > 0$, ground states with substantially overlapping components are expected, whereas for $\Delta_{\text{misc}} < 0$, the components are mostly separated in space according to the Gross–Pitaevskii model; see, e.g., [58]. In this paper, we focus on the regime where $\Delta_{\text{misc}} > 0$.

We are interested in global minimisers of the energy (1.2) subject to the mass constraints (1.1) on the components. These minimisers are the ground states that represent the most stable configurations of the system. The existence of a ground state for $p = 2$ in the full-space problem has been shown in [14]. Building on the approach used to establish the existence and uniqueness in the single-component case [23, 48], we extend these results to general p and bounded domains under suitable assumptions on the potentials V_j and the interaction matrix $K = [\kappa_{ij}]_{i,j=1}^p$.

The ground state of a multicomponent BEC with p interacting components is further characterised as the solution to the nonlinear eigenvector problem (NLEVP) given by the coupled (dimensionless) Gross–Pitaevskii equations

$$(1.3) \quad -\Delta\varphi_j + V_j\varphi_j + \rho_j(\boldsymbol{\varphi})\varphi_j = \lambda_j\varphi_j, \quad j = 1, \dots, p,$$

where the eigenvalues $\lambda_1, \dots, \lambda_p \in \mathbb{R}$ represent the chemical potentials of the components. We show that, similar to the single-component case [23], each component of the ground state is associated with the eigenfunction corresponding to the smallest eigenvalue for the corresponding condensate component. This relationship is crucial in proving both the uniqueness of the ground state, up to a global sign change of its components, and a second-order necessary optimality condition.

Various numerical methods have been proposed for computing ground states of the Gross–Pitaevskii equation in the single-component case, based on either energy minimisation or eigenvalue characterisation. These methods include self-consistent field iterations [24, 31], discrete normalised gradient flows [17, 19], (projected) Sobolev gradient methods [28, 29, 36, 41, 45], the J -method [5, 44], Riemannian optimisation methods in both discrete and continuous settings [9, 12, 30], and Newton-type methods [20, 32, 60]. For more details and an extended overview, we refer to [39]. Although the computation of ground states for multicomponent BECs is also important in practice, it has received significantly less attention. Among the methods proposed for these problems are gradient flow-based approaches [10, 13], a Newton-like method with an approximate line search strategy [22], and more recently Newton-based alternating methods [43].

This paper promotes Riemannian gradient descent and Newton-type methods for multicomponent BECs, emphasising their robustness across different spatial discretisation methods by working within an infinite-dimensional framework. Consequently, the convergence properties of selected optimisation schemes are asymptotically independent when the resolution in the spatial discretisation is increased, such as mesh refinement in finite element methods. In contrast, conventional convergence proofs in Riemannian optimisation for discrete models often lack an explicit dependence on the dimension of the problem, limiting their applicability to discretised partial differential equations where the dimension is critical and increases with increasing spatial resolution. Furthermore, we provide a rigorous global convergence analysis and quantify the local convergence behaviour of a selected Riemannian gradient descent scheme, demonstrating its effectiveness in reliably identifying accurate initial values for empirically more efficient Riemannian Newton methods within sufficiently close neighbourhoods of the ground state.

The paper is organised as follows. Section 2 introduces the functional analytical framework for constrained energy minimisation and proves the existence of a ground state. Section 3 establishes the connection to NLEVPs and shows the uniqueness of the ground state. In Section 4, we characterise the tangent and normal spaces of the infinite-dimensional generalised oblique manifold, deriving formulae for Riemannian gradients and Hessians based on the chosen metric. Section 5 presents

the Riemannian gradient descent and Newton methods, followed by the convergence analysis of the energy-adaptive Riemannian gradient descent method in Section 6. Section 7 discusses the finite element discretisation and the discrete geometric ingredients. Finally, Section 8 reports on numerical experiments.

Notation. The set of $p \times p$ real diagonal matrices is denoted by $\mathcal{D}(p)$. For $M \in \mathbb{R}^{p \times p}$, the trace of M is denoted by $\text{trace } M$. In addition, we denote by $\text{diag}(v)$ the diagonal matrix with components of a vector $v \in \mathbb{R}^p$ on the diagonal and by $\text{ddiag}(M)$ the diagonal matrix whose diagonal elements are the same as that of M . The $p \times p$ identity and zero matrices are denoted by I_p and 0_p , respectively. The Euclidean vector norm is denoted by $\|\cdot\|$ and the spectral matrix norm is denoted by $\|\cdot\|_2$.

2. CONSTRAINED ENERGY MINIMISATION AND EXISTENCE OF A GROUND STATE

The ground states are precisely defined by a mathematical model of constrained energy minimisation. Their existence is then proved under appropriate assumptions on the model parameters.

2.1. Energy-related mathematical model. Let $\Omega \subset \mathbb{R}^d$ with $d = 1, 2, 3$ be a bounded convex Lipschitz domain. Consider the Hilbert space $L^2(\Omega)$ with the inner product $(\cdot, \cdot)_{L^2(\Omega)}$ and the Sobolev space $H_0^1(\Omega)$ with the inner product $(\cdot, \cdot)_{H_0^1(\Omega)}$. For $p \geq 1$, we define the Hilbert spaces $L = [L^2(\Omega)]^p$ and $H = [H_0^1(\Omega)]^p$ of p -frames which form a Gelfand triple $H \subset L \subset H^*$, where $H^* = [H^{-1}(\Omega)]^p$ denotes the dual space of H . On the pivot space L , we define an inner product

$$(\mathbf{v}, \mathbf{w})_L = \sum_{j=1}^p (v_j, w_j)_{L^2(\Omega)}$$

for $\mathbf{v} = (v_1, \dots, v_p), \mathbf{w} = (w_1, \dots, w_p) \in L$, which induces the norm $\|\mathbf{v}\|_L = \sqrt{(\mathbf{v}, \mathbf{v})_L}$. In addition, we introduce the diagonal matrix

$$\langle\langle \mathbf{v}, \mathbf{w} \rangle\rangle = \text{diag}((v_1, w_1)_{L^2(\Omega)}, \dots, (v_p, w_p)_{L^2(\Omega)})$$

of the component-wise L^2 -inner products of $\mathbf{v}, \mathbf{w} \in L$. Due to the symmetry of the L^2 -inner product, we have $\langle\langle \mathbf{v}, \mathbf{w} \rangle\rangle = \langle\langle \mathbf{w}, \mathbf{v} \rangle\rangle$. Moreover, it holds $(\mathbf{v}, \mathbf{w})_L = \text{trace } \langle\langle \mathbf{v}, \mathbf{w} \rangle\rangle$.

We consider the energy functional $\mathcal{E}: H \rightarrow \mathbb{R}$ from (1.2), which can also be written as

$$(2.1) \quad \mathcal{E}(\boldsymbol{\varphi}) = \int_{\Omega} \frac{1}{2} \text{trace}((\nabla \boldsymbol{\varphi})^T \nabla \boldsymbol{\varphi}) + \frac{1}{2}(\boldsymbol{\varphi} \circ \boldsymbol{\varphi})V(x) + \frac{1}{4}(\boldsymbol{\varphi} \circ \boldsymbol{\varphi})K(\boldsymbol{\varphi} \circ \boldsymbol{\varphi})^T dx,$$

where $\boldsymbol{\varphi} \circ \mathbf{v} = (\varphi_1 v_1, \dots, \varphi_p v_p)$ denotes the Hadamard (component-wise) product of two p -frames, $V = [V_1, \dots, V_p]^T$, and $K = [\kappa_{ij}]_{i,j=1}^p \in \mathbb{R}^{p \times p}$. Our aim is to compute a global minimiser of \mathcal{E} , a so-called *ground state*, on the manifold

$$(2.2) \quad \mathcal{OB}_N(p, H) = \{\boldsymbol{\varphi} \in H : \langle\langle \boldsymbol{\varphi}, \boldsymbol{\varphi} \rangle\rangle = N\}$$

of admissible states that respect the prescribed masses of the individual components, encoded in the diagonal matrix $N = \text{diag}(N_1, \dots, N_p)$; see also (1.1). This manifold is known as the *infinite-dimensional generalised oblique manifold*. The resulting constrained energy minimisation problem can then shortly be written as

$$(2.3) \quad \min_{\boldsymbol{\varphi} \in \mathcal{OB}_N(p, H)} \mathcal{E}(\boldsymbol{\varphi}).$$

For simplicity, the restriction of \mathcal{E} to $\mathcal{OB}_N(p, H)$ will also be denoted by \mathcal{E} in what follows.

Remark 2.1 (Scaling invariance of \mathcal{E} and non-uniqueness of ground state). The energy functional satisfies $\mathcal{E}(\boldsymbol{\varphi} \Sigma_{\pm 1}) = \mathcal{E}(\boldsymbol{\varphi})$ for all $\boldsymbol{\varphi} \in \mathcal{OB}_N(p, H)$ and $\Sigma_{\pm 1} \in \mathcal{D}(p)$ with ± 1 on the diagonal. Thus, any global or local minimiser of (2.3), if it exists, is not unique in the strict sense. A proper concept of uniqueness will be introduced later in Section 3.

Throughout this paper, we make the following assumptions on the model parameters V_j and K :

A1: The external potentials satisfy $V_j \in L^\infty(\Omega)$ with $V_j(x) \geq 0$ for almost all $x \in \Omega$.

A2: The interaction matrix K is symmetric and positive definite.

Assumption **A1** allows us to equip the space H with the potential-dependent inner product

$$(\mathbf{v}, \mathbf{w})_H = \sum_{j=1}^p \int_{\Omega} (\nabla v_j)^T \nabla w_j + V_j(x) v_j w_j \, dx$$

and the induced norm $\|\mathbf{v}\|_H = \sqrt{(\mathbf{v}, \mathbf{v})_H}$, which is equivalent to the canonical norm of H . Note that, for $p = 2$, Assumption **A2** corresponds to the miscible regime $\Delta_{\text{misc}} > 0$. In Section 2.3 below, we show that these assumptions ensure the existence of a ground state. In the proof and throughout the paper, we will frequently use several Sobolev embedding inequalities [53, Sec. 7.10.4.],

$$(2.4) \quad d \geq 1 : \quad \|\mathbf{v}\|_{[L^2(\Omega)]^p} \leq C_2 \|\mathbf{v}\|_H \quad \text{for all } \mathbf{v} \in H,$$

$$(2.5) \quad d \leq 3 : \quad \|\mathbf{v}\|_{[L^4(\Omega)]^p} \leq C_4 \|\mathbf{v}\|_H \quad \text{for all } \mathbf{v} \in H,$$

$$(2.6) \quad d = 3 : \quad \|\mathbf{v}\|_{[L^6(\Omega)]^p} \leq C_6 \|\mathbf{v}\|_H \quad \text{for all } \mathbf{v} \in H,$$

with constants $C_2, C_4, C_6 > 0$.

2.2. Properties of the derivative of the energy. The energy functional \mathcal{E} is Fréchet differentiable on H . Its directional derivative at $\boldsymbol{\varphi} \in H$ along $\mathbf{w} \in H$ is given by

$$D\mathcal{E}(\boldsymbol{\varphi})[\mathbf{w}] = a_{\boldsymbol{\varphi}}(\boldsymbol{\varphi}, \mathbf{w})$$

with the bilinear form $a_{\boldsymbol{\varphi}}: H \times H \rightarrow \mathbb{R}$,

$$(2.7) \quad \begin{aligned} a_{\boldsymbol{\varphi}}(\mathbf{v}, \mathbf{w}) &= \sum_{j=1}^p \int_{\Omega} (\nabla v_j)^T \nabla w_j + V_j(x) v_j w_j + \rho_j(\boldsymbol{\varphi}) v_j w_j \, dx \\ &= \int_{\Omega} \text{trace}((\nabla \mathbf{v})^T \nabla \mathbf{w}) + (\mathbf{v} \circ \mathbf{w})V(x) + (\boldsymbol{\varphi} \circ \boldsymbol{\varphi})K(\mathbf{v} \circ \mathbf{w})^T \, dx. \end{aligned}$$

The following lemma establishes some useful properties of $a_{\boldsymbol{\varphi}}$.

Proposition 2.2. *Consider $\boldsymbol{\varphi} \in H$ and let Assumption **A1** be fulfilled. Then the bilinear form $a_{\boldsymbol{\varphi}}$ defined in (2.7) is symmetric, bounded, and satisfies a Gårding inequality.*

Proof. The proofs of symmetry and boundedness are straightforward. In order to prove the Gårding inequality for $d = 3$, we first observe that the interpolation inequality [33, App. B2] and the Sobolev embedding inequality (2.6) imply that

$$(2.8) \quad \|\mathbf{v}\|_{[L^4(\Omega)]^p} \leq \|\mathbf{v}\|_L^{1/4} \|\mathbf{v}\|_{[L^6(\Omega)]^p}^{3/4} \leq C_6^{3/4} \|\mathbf{v}\|_L^{1/4} \|\mathbf{v}\|_H^{3/4}.$$

Using the Cauchy–Schwarz and Hölder inequalities (see, e.g., [33, App. B2]) as well as (2.8), we then obtain

$$\begin{aligned} \|\mathbf{v}\|_H^2 &= a_{\boldsymbol{\varphi}}(\mathbf{v}, \mathbf{v}) - \int_{\Omega} (\boldsymbol{\varphi} \circ \boldsymbol{\varphi})K(\mathbf{v} \circ \mathbf{v})^T \, dx \leq a_{\boldsymbol{\varphi}}(\mathbf{v}, \mathbf{v}) + \|K\|_2 \|\boldsymbol{\varphi} \circ \boldsymbol{\varphi}\|_L \|\mathbf{v} \circ \mathbf{v}\|_L \\ &\leq a_{\boldsymbol{\varphi}}(\mathbf{v}, \mathbf{v}) + C_6^{3/2} \|K\|_2 \|\boldsymbol{\varphi}\|_{[L^4(\Omega)]^p}^2 \|\mathbf{v}\|_L^{1/2} \|\mathbf{v}\|_H^{3/2}. \end{aligned}$$

Applying Young’s inequality [33, App. B2] twice, we get

$$\begin{aligned} C_6^{3/2} \|K\|_2 \|\boldsymbol{\varphi}\|_{[L^4(\Omega)]^p}^2 \|\mathbf{v}\|_L^{1/2} \|\mathbf{v}\|_H^{3/2} &= 2 (C_6^{3/2} \|K\|_2 \|\boldsymbol{\varphi}\|_{[L^4(\Omega)]^p}^2 \|\mathbf{v}\|_L^{1/2} \|\mathbf{v}\|_H^{1/2}) \left(\frac{1}{2} \|\mathbf{v}\|_H\right) \\ &\leq C_6^3 \|K\|_2^2 \|\boldsymbol{\varphi}\|_{[L^4(\Omega)]^p}^4 \|\mathbf{v}\|_L \|\mathbf{v}\|_H + \frac{1}{4} \|\mathbf{v}\|_H^2 \\ &\leq C_6^6 \|K\|_2^4 \|\boldsymbol{\varphi}\|_{[L^4(\Omega)]^p}^8 \|\mathbf{v}\|_L^2 + \frac{1}{2} \|\mathbf{v}\|_H^2. \end{aligned}$$

Finally, combining the previous inequalities implies the Gårding inequality

$$a_{\boldsymbol{\varphi}}(\mathbf{v}, \mathbf{v}) \geq \frac{1}{2} \|\mathbf{v}\|_H^2 - C_6^6 \|K\|_2^4 \|\boldsymbol{\varphi}\|_{[L^4(\Omega)]^p}^8 \|\mathbf{v}\|_L^2.$$

For $d = 2$, a similar argument can be made using the Ladyzhenskaya inequality [47],

$$\|\mathbf{v}\|_{[L^4(\Omega)]^p} \leq C_L \|\mathbf{v}\|_L^{1/2} \|\nabla \mathbf{v}\|_L^{1/2} \leq C_L \|\mathbf{v}\|_L^{1/2} \|\mathbf{v}\|_H^{1/2}$$

with a constant $C_L > 0$. For $d = 1$, we can directly apply the embedding $H_0^1(\Omega) \hookrightarrow L^\infty(\Omega)$. \square

Remark 2.3 (Coercivity of a_φ for non-negative K). If all entries in the interaction matrix K are non-negative, then the integrand $(\varphi \circ \varphi)K(\mathbf{v} \circ \mathbf{v})^T$ in the nonlinear term of $a_\varphi(\mathbf{v}, \mathbf{v})$ is non-negative almost everywhere. Hence, a_φ is coercive with a coercivity constant of 1, which means that for all $\mathbf{v} \in H$, we have $a_\varphi(\mathbf{v}, \mathbf{v}) \geq \|\mathbf{v}\|_H^2$.

In the remainder of this paper, we assume without loss of generality that the bilinear form a_φ is coercive. If this is not the case, based on Proposition 2.2, we replace it by $a_\varphi(\mathbf{v}, \mathbf{w}) + C_\varphi(\mathbf{v}, \mathbf{w})_L$ with an appropriately chosen constant $C_\varphi > 0$, which may depend on φ . In terms of the minimisation problem, this corresponds to a (constant) shift of the external potentials V_j by C_φ . Due to the constraint imposed by the generalised oblique manifold, this translates into a constant shift in energy that does not affect the minimisers of (2.3).

For any fixed $\varphi \in H$, the coercive bilinear form a_φ defines another inner product on H and induces the norm $\|\mathbf{v}\|_{a_\varphi} = \sqrt{a_\varphi(\mathbf{v}, \mathbf{v})}$, which is equivalent to the H -norm in the sense that there exists a constant $C_H > 0$ such that for all $\mathbf{v} \in H$,

$$C_H \|\mathbf{v}\|_{a_\varphi} \leq \|\mathbf{v}\|_H \leq \|\mathbf{v}\|_{a_\varphi}.$$

Moreover, the bilinear form a_φ defines the *Gross–Pitaevskii Hamiltonian* $\mathcal{A}_\varphi: H \rightarrow H^*$ given by

$$(2.9) \quad \langle \mathcal{A}_\varphi \mathbf{v}, \mathbf{w} \rangle = a_\varphi(\mathbf{v}, \mathbf{w}) \quad \text{for all } \mathbf{v}, \mathbf{w} \in H,$$

where $\langle \cdot, \cdot \rangle$ denotes the duality pairing on $H^* \times H$. In particular, we have $D\mathcal{E}(\varphi)[\mathbf{w}] = \langle \mathcal{A}_\varphi \varphi, \mathbf{w} \rangle$ for all $\mathbf{w} \in H$. The coercivity property of the bilinear form a_φ further implies the existence of the inverse operator $\mathcal{A}_\varphi^{-1}: H^* \rightarrow H$. Throughout this paper, this operator will mostly be applied to functions in H , which is well-defined due to the canonical inclusion $H \subseteq H^*$.

Due to the additive structure of a_φ in (2.7), the operator \mathcal{A}_φ can be represented as

$$(2.10a) \quad \langle \mathcal{A}_\varphi \mathbf{v}, \mathbf{w} \rangle = \sum_{j=1}^p \langle \mathcal{A}_{\varphi,j} v_j, w_j \rangle \quad \text{for all } \mathbf{v}, \mathbf{w} \in H,$$

where the component operators $\mathcal{A}_{\varphi,j}: H_0^1(\Omega) \rightarrow H^{-1}(\Omega)$ are given by

$$(2.10b) \quad \langle \mathcal{A}_{\varphi,j} v_j, w_j \rangle = \int_{\Omega} (\nabla v_j)^T \nabla w_j + V_j(x) v_j w_j + \rho_j(\varphi) v_j w_j \, dx, \quad j = 1, \dots, p.$$

Note that, for fixed φ , the operator $\mathcal{A}_{\varphi,j}$ is simply the weak form of the Laplacian shifted by a bounded potential $V_j + \rho_j(\varphi)$. Formula (2.10a) shows that the operator \mathcal{A}_φ acts component-wise on a p -frame, i.e.,

$$(2.11) \quad \mathcal{A}_\varphi \mathbf{v} = (\mathcal{A}_{\varphi,1} v_1, \dots, \mathcal{A}_{\varphi,p} v_p).$$

Hence, for all $\mathbf{v} \in H$ and $\Lambda \in \mathcal{D}(p)$, we have $\mathcal{A}_\varphi(\mathbf{v}\Lambda) = (\mathcal{A}_\varphi \mathbf{v})\Lambda$. Such properties are also present in the Hartree–Fock and Kohn–Sham Hamiltonians studied in [8, 54]. Unlike these Hamiltonians, however, the individual operators $\mathcal{A}_{\varphi,j}$ in (2.11) vary between the components, making the analysis of multicomponent BECs more difficult.

2.3. Existence of a ground state. The following theorem generalises the existence of ground states for two-component BECs from [14, Th. 2.6] to the multicomponent case. However, even in the case $p = 2$, there are slight differences in the assumptions. Specifically, [14] considers the entire space \mathbb{R}^d , whereas we focus on bounded spatial domains.

Theorem 2.4 (Existence of a ground state). *Let Assumptions **A1** and **A2** be satisfied. Then there exists a ground state $\varphi_* \in \mathcal{OB}_N(p, H)$, i.e., a global minimiser of the constrained minimisation problem (2.3).*

Proof. The proof essentially follows the approach of [23, Lem. 2], to which we refer for details that we omit here for the sake of brevity. Due to Assumptions **A1** and **A2**, the energy functional \mathcal{E} in (2.1) is bounded from below (by zero). Hence, there exists a minimising sequence φ^n in $\mathcal{OB}_N(p, H) \subset H$. Since this sequence is bounded in H , there exists a weak limit $\varphi^\infty \in H$ such that (up to a subsequence) for each component, we have

$$\varphi_j^n \rightharpoonup \varphi_j^\infty \text{ in } H_0^1(\Omega), \quad j = 1, \dots, p.$$

The compact embedding $H_0^1(\Omega) \hookrightarrow L^2(\Omega)$ then implies strong convergence $\varphi_j^n \rightarrow \varphi_j^\infty$ of the components in $L^2(\Omega)$ and hence

$$\|\varphi_j^\infty\|_{L^2(\Omega)}^2 = \lim_{n \rightarrow \infty} \|\varphi_j^n\|_{L^2(\Omega)}^2 = N_j, \quad j = 1, \dots, p,$$

proving the feasibility of $\varphi^\infty \in \mathcal{OB}_N(p, H)$. The weak lower semi-continuity of the functional \mathcal{E} on H shows that $\varphi_* = \varphi^\infty$ is a global minimiser. \square

Remark 2.5 (Non-negative ground state). Analogously to the proof of [48, Th. A.4], we have that if $\varphi_* \in \mathcal{OB}_N(p, H)$, then $|\varphi_*| \in \mathcal{OB}_N(p, H)$ and $\mathcal{E}(|\varphi_*|) \leq \mathcal{E}(\varphi_*)$, where $|\varphi_*|$ is the p -frame with absolute values in the components. This implies that with φ_* also $|\varphi_*|$ is a ground state. Hence, there exists a non-negative ground state $\varphi_* \geq 0$, where the inequality is understood to be component-wise.

3. NONLINEAR EIGENVECTOR PROBLEM AND UNIQUENESS OF THE GROUND STATE

This section aims to derive the necessary first-order and second-order optimality conditions of the ground state. In particular, we will characterise the constrained critical points of the energy as solutions to the NLEVP (1.3) representing the critical points of the Lagrangian.

3.1. Critical points and nonlinear eigenvector problem. To establish a relation between the coupled Gross–Pitaevskii eigenvalue problem (1.3) and the energy minimisation problem (2.3), we consider the Lagrange functional

$$(3.1) \quad \mathcal{L}(\varphi, \Lambda) = \mathcal{E}(\varphi) - \frac{1}{2} \text{trace} \left(\Lambda (\langle\langle \varphi, \varphi \rangle\rangle - N) \right)$$

with a Lagrange multiplier $\Lambda \in \mathcal{D}(p)$. The directional derivative of \mathcal{L} with respect to $\varphi \in H$ along $\mathbf{w} \in H$ is given by

$$D_\varphi \mathcal{L}(\varphi, \Lambda)[\mathbf{w}] = D\mathcal{E}(\varphi)[\mathbf{w}] - (\varphi \Lambda, \mathbf{w})_L = \langle \mathcal{A}_\varphi \varphi, \mathbf{w} \rangle - (\varphi \Lambda, \mathbf{w})_L.$$

A p -frame $\varphi \in H$ is called a *constrained critical point* of the energy functional \mathcal{E} if $\varphi \in \mathcal{OB}_N(p, H)$ is feasible and if it is a critical point of the Lagrangian, i.e., there exists a Lagrange multiplier $\Lambda \in \mathcal{D}(p)$ such that $D_\varphi \mathcal{L}(\varphi, \Lambda)[\mathbf{w}] = 0$ for all $\mathbf{w} \in H$, or, equivalently,

$$(3.2) \quad \langle \mathcal{A}_\varphi \varphi, \mathbf{w} \rangle = (\varphi \Lambda, \mathbf{w})_L \quad \text{for all } \mathbf{w} \in H.$$

Note in particular that a ground state φ_* is a constrained critical point of \mathcal{E} . The computation of critical points for the constrained energy minimisation problem (2.3) is therefore linked to the NLEVP (3.2). Using (2.10a), the NLEVP (3.2) can equivalently be written component-wise as

$$(3.3) \quad \langle \mathcal{A}_{\varphi, j} \varphi_j, w_j \rangle = \lambda_j (\varphi_j, w_j)_{L^2(\Omega)} \quad \text{for all } w_j \in H_0^1(\Omega).$$

This equals the weak formulation of the coupled Gross–Pitaevskii eigenvalue problem previously stated in (1.3). Given a pair consisting of a p -frame φ and a diagonal matrix $\Lambda = \text{diag}(\lambda_1, \dots, \lambda_p)$ that solves (3.2), we call φ an *eigenvector* corresponding to *eigenvalues* $\lambda_1, \dots, \lambda_p$.

For a constrained critical point $\varphi \in \mathcal{OB}_N(p, H)$, the corresponding Lagrange multiplier Λ can be determined as $\Lambda = \langle\langle \mathcal{A}_\varphi \varphi, \varphi \rangle\rangle N^{-1}$, which is well-defined due to the assumed Gelfand triple $H \subset L \subset H^*$. This particularly implies that the diagonal entries λ_j of Λ are given by the Rayleigh quotients

$$\lambda_j = \frac{\langle \mathcal{A}_{\varphi, j} \varphi_j, \varphi_j \rangle}{(\varphi_j, \varphi_j)_{L^2(\Omega)}}, \quad j = 1, \dots, p,$$

of the component operators $\mathcal{A}_{\varphi, j}$.

Lemma 3.1 (Eigenvalues and eigenfunctions of $\mathcal{A}_{\varphi, j}$). Let Assumption **A1** be fulfilled. Then for fixed $\varphi \in \mathcal{OB}_N(p, H)$ and $j = 1, \dots, p$, the operator $\mathcal{A}_{\varphi, j}$ introduced in (2.10b) has an L^2 -orthogonal basis of eigenfunctions $v_{j,1}, v_{j,2}, \dots$ in $H_0^1(\Omega)$ corresponding to the real eigenvalues $\lambda_1(\mathcal{A}_{\varphi, j}) < \lambda_2(\mathcal{A}_{\varphi, j}) \leq \dots$ ordered increasingly. Furthermore, the smallest eigenvalue $\lambda_1(\mathcal{A}_{\varphi, j})$ is simple and the corresponding eigenfunction satisfies $|v_{j,1}| > 0$ in Ω .

Proof. For fixed $\varphi \in \mathcal{OB}_N(p, H)$, the operator $\mathcal{A}_{\varphi,j}$ corresponds to the linear Schrödinger operator with external potential $V_j + \rho_j(\varphi)$. By Proposition 2.2, we know that there exists a constant $C_\varphi > 0$ such that $a_{\varphi,j}(v, w) := \langle \mathcal{A}_{\varphi,j}v, w \rangle + C_\varphi(v, w)_{L^2(\Omega)}$ defines a symmetric, bounded, and coercive bilinear form. This implies that $\mathcal{A}_{\varphi,j} = \mathcal{A}_{|\varphi|,j}$ has a countably infinite number of real eigenvalues such that the smallest eigenvalue is simple. The corresponding eigenfunctions form an L^2 -orthogonal basis in $H_0^1(\Omega)$. Moreover, according to the proof of [23, Lem. 2], $v_{j,1}$ is Hölder continuous and can be chosen to be positive in Ω . \square

The subsequent result connects the eigenvalues of the component operators with the diagonal elements of the Lagrange multiplier corresponding to the ground state.

Proposition 3.2 (Characterisation of Lagrange multipliers as eigenvalues of components). *Let Assumptions A1 and A2 be fulfilled and let $\varphi_* \in \mathcal{OB}_N(p, H)$ with $\varphi_* \geq 0$ be a ground state of the energy functional \mathcal{E} in (1.2) with the Lagrange multiplier $\Lambda_* = \text{diag}(\lambda_{*,1}, \dots, \lambda_{*,p})$. Then, for all $j = 1, \dots, p$, the smallest eigenvalue $\lambda_1(\mathcal{A}_{\varphi_*,j})$ of $\mathcal{A}_{\varphi_*,j}$ coincides with $\lambda_{*,j}$, i.e., $\lambda_1(\mathcal{A}_{\varphi_*,j}) = \lambda_{*,j}$.*

Proof. For a ground state $\varphi_* = (\varphi_{*,1}, \dots, \varphi_{*,p}) \in \mathcal{OB}_N(p, H)$ with $\varphi_* \geq 0$, we obtain from (3.3) that $\lambda_{*,j}$ is an eigenvalue of the operator $\mathcal{A}_{\varphi_*,j}$ and $\varphi_{*,j}$ is the corresponding eigenfunction. Then the required result follows from the proof of [23, Lem. 2]. \square

3.2. Uniqueness of the ground state. Given that the ground state as a global minimiser of (2.3) is also an eigenvector of the NLEVP (3.2) with component-wise minimality properties as established in Proposition 3.2, we can now state a uniqueness result for the ground state.

Theorem 3.3 (Uniqueness of the ground state). *Let Assumptions A1 and A2 be fulfilled. Then the ground state is unique up to the global signs of its components. We can, therefore, choose the ground state φ_* to be component-wise positive in Ω .*

Proof. Similarly to the single-component case [23, 48], we introduce a convex problem by considering the modified functional $\mathcal{E}(\sqrt{\bullet})$ acting on the convex set of densities

$$\Upsilon = \{\boldsymbol{\rho} \in L : \boldsymbol{\rho} \geq 0 \text{ and } \sqrt{\boldsymbol{\rho}} \in \mathcal{OB}_N(p, H)\},$$

where $\boldsymbol{\rho} \geq 0$ means that all components of $\boldsymbol{\rho}$ are non-negative point-wise almost everywhere, and the square root is taken component-wise. Given $\boldsymbol{\rho}^{[1]}, \boldsymbol{\rho}^{[2]} \in \Upsilon$, define $\varphi^{[i]} = \sqrt{\boldsymbol{\rho}^{[i]}} \in \mathcal{OB}_N(p, H)$ for $i = 1, 2$. First note that $\varphi = (\varphi_1, \dots, \varphi_p)$ with components

$$\varphi_j = \sqrt{\alpha \rho_j^{[1]} + (1 - \alpha) \rho_j^{[2]}}, \quad \alpha \in (0, 1),$$

satisfies $\langle \varphi, \varphi \rangle = N$ and, hence, $\varphi \in \mathcal{OB}_N(p, H)$. Hence, [48, Lem. A.1] implies that

$$\|\nabla \varphi_j\|^2 \leq \alpha \|\nabla \varphi_j^{[1]}\|^2 + (1 - \alpha) \|\nabla \varphi_j^{[2]}\|^2, \quad j = 1, \dots, p.$$

Therefore, the first term of $\mathcal{E}(\sqrt{\bullet})$ involving the gradients is convex on Υ . In addition, the second term containing the potential V is linear and the last term with the positive definite interaction matrix K is quadratic. As the sum of three (strictly) convex functionals, $\mathcal{E}(\sqrt{\bullet})$ is therefore strictly convex on the convex set Υ . For $\varphi_* \geq 0$, its density $\boldsymbol{\rho}_* = \varphi_* \circ \varphi_* \in \Upsilon$ minimises the functional $\mathcal{E}(\sqrt{\bullet})$ on Υ . The strict convexity of $\mathcal{E}(\sqrt{\bullet})$ on the convex feasible set Υ , as shown above, implies the uniqueness of the density. By Lemma 3.1, the components of any ground state have no sign change in Ω by a maximum principle. This, in turn, shows that the only remaining degree of freedom is a global sign change in the components, which is the strongest possible form of uniqueness according to Remark 2.1. \square

Based on Proposition 3.2, under Assumptions A1 and A2, the unique positive ground state φ_* is an eigenvector of the NLEVP (3.2) corresponding to the p smallest eigenvalues $\lambda_{*,1}, \dots, \lambda_{*,p}$ of the component operators $\mathcal{A}_{\varphi_*,1}, \dots, \mathcal{A}_{\varphi_*,p}$, respectively. There exists a spectral gap in the following sense.

Remark 3.4 (Spectral gap). Generalising the proof for the single-component case given in [23, p. 117] to the multicomponent case, one can show that if $\varphi \in \mathcal{OB}_N(p, H)$ is an eigenvector of the NLEVP (3.2) corresponding to the eigenvalues $\lambda_1, \dots, \lambda_p$, then either $\lambda_j = \lambda_{*,j}$ for $j = 1, \dots, p$ and $\varphi = \varphi_* \Sigma_{\pm 1}$, or there exists an index $j_0 \in \{1, \dots, p\}$ such that $\lambda_{j_0} > \lambda_{*,j_0}$.

3.3. Second-order derivatives and optimality condition. The second (directional) derivative of \mathcal{E} at φ in the direction of $\mathbf{v}, \mathbf{w} \in H$ can be computed as

$$(3.4) \quad D^2 \mathcal{E}(\varphi)[\mathbf{v}, \mathbf{w}] = \lim_{t \rightarrow 0} \frac{1}{t} \langle \mathcal{A}_{\varphi+t\mathbf{v}}(\varphi + t\mathbf{v}) - \mathcal{A}_{\varphi} \varphi, \mathbf{w} \rangle = \langle \mathcal{A}_{\varphi} \mathbf{v} + \mathcal{B}_{\varphi}(\mathbf{v}, \varphi), \mathbf{w} \rangle,$$

where the operator $\mathcal{B}_{\varphi}: H \times H \rightarrow H^*$ is given by

$$(3.5a) \quad \langle \mathcal{B}_{\varphi}(\mathbf{v}, \mathbf{u}), \mathbf{w} \rangle = \sum_{i,j=1}^p \langle \mathcal{B}_{\varphi,ij}(v_i, u_j), w_j \rangle \quad \text{for all } \mathbf{u}, \mathbf{v}, \mathbf{w} \in H$$

with

$$(3.5b) \quad \langle \mathcal{B}_{\varphi,ij}(v_i, u_j), w_j \rangle = 2 \int_{\Omega} \kappa_{ij} \varphi_i v_i u_j w_j \, dx, \quad i, j = 1, \dots, p.$$

Similar to (2.1), we can also express \mathcal{B}_{φ} compactly as

$$(3.6) \quad \langle \mathcal{B}_{\varphi}(\mathbf{v}, \mathbf{u}), \mathbf{w} \rangle = 2 \int_{\Omega} (\varphi \circ \mathbf{v}) K(\mathbf{u} \circ \mathbf{w})^T \, dx.$$

We now turn to the second-order derivative of the Lagrangian \mathcal{L} in (3.1) with respect to the first variable. It reads

$$(3.7) \quad \begin{aligned} D_{\varphi\varphi}^2 \mathcal{L}(\varphi, \Lambda)[\mathbf{v}, \mathbf{w}] &= D^2 \mathcal{E}(\varphi)[\mathbf{v}, \mathbf{w}] - (\mathbf{v} \Lambda, \mathbf{w})_L \\ &= \langle \mathcal{A}_{\varphi} \mathbf{v}, \mathbf{w} \rangle + \langle \mathcal{B}_{\varphi}(\mathbf{v}, \varphi), \mathbf{w} \rangle - (\mathbf{v} \Lambda, \mathbf{w})_L, \quad \mathbf{v}, \mathbf{w} \in H. \end{aligned}$$

The following theorem presents a second-order necessary optimality condition by showing that the second-order derivative of the Lagrangian at a ground state is positive definite on the tangent space to the set of constraints described by (1.1).

Theorem 3.5 (Second-order necessary optimality condition). *Let Assumptions **A1** and **A2** be fulfilled and let $\varphi_* \in \mathcal{OB}_N(p, H)$ with $\varphi_* \geq 0$ be a ground state of \mathcal{E} with the corresponding Lagrange multiplier $\Lambda_* = \langle \langle \varphi_*, \mathcal{A}_{\varphi_*} \varphi_* \rangle \rangle N^{-1}$. Then*

$$D_{\varphi\varphi}^2 \mathcal{L}(\varphi_*, \Lambda_*)[\mathbf{z}, \mathbf{z}] > 0$$

for all nonzero $\mathbf{z} \in H$ such that $\langle \langle \varphi_*, \mathbf{z} \rangle \rangle = 0$.

Proof. Let $\varphi_* = (\varphi_{*,1}, \dots, \varphi_{*,p}) \geq 0$ be a ground state of the functional \mathcal{E} with the Lagrange multiplier $\Lambda_* = \text{diag}(\lambda_{*,1}, \dots, \lambda_{*,p})$. Furthermore, let $v_{j,1}, v_{j,2}, \dots$ be the eigenfunctions of $\mathcal{A}_{\varphi_*,j}$ which form an L^2 -orthogonal basis of $H_0^1(\Omega)$ and let $\lambda_1(\mathcal{A}_{\varphi_*,j}) < \lambda_2(\mathcal{A}_{\varphi_*,j}) \leq \dots$ be the corresponding eigenvalues. By Proposition 3.2, we know that $v_{j,1} = \pm \varphi_{*,j}$ and $\lambda_1(\mathcal{A}_{\varphi_*,j}) = \lambda_{*,j}$ for $j = 1, \dots, p$. For any $\mathbf{z} \in H$, we obtain from Assumption **A2** and the relation (3.6) that $\langle \mathcal{B}_{\varphi_*}(\mathbf{z}, \varphi_*), \mathbf{z} \rangle \geq 0$. Together with (3.7), this yields

$$\begin{aligned} D_{\varphi\varphi}^2 \mathcal{L}(\varphi_*, \Lambda_*)[\mathbf{z}, \mathbf{z}] &= \langle \mathcal{A}_{\varphi_*} \mathbf{z}, \mathbf{z} \rangle + \langle \mathcal{B}_{\varphi_*}(\mathbf{z}, \varphi_*), \mathbf{z} \rangle - (\mathbf{z} \Lambda_*, \mathbf{z})_L \\ &\geq \langle \mathcal{A}_{\varphi_*} \mathbf{z}, \mathbf{z} \rangle - \text{trace} \langle \langle \mathbf{z} \Lambda_*, \mathbf{z} \rangle \rangle. \end{aligned}$$

If $\langle \langle \varphi_*, \mathbf{z} \rangle \rangle = 0$, then each component z_j of \mathbf{z} can be represented as $z_j = \sum_{\ell \geq 2} \alpha_{j,\ell} v_{j,\ell}$ with $\alpha_{j,\ell} \in \mathbb{R}$. For nonzero \mathbf{z} , this finally implies that

$$\begin{aligned} D_{\varphi\varphi}^2 \mathcal{L}(\varphi_*, \Lambda_*)[\mathbf{z}, \mathbf{z}] &\geq \sum_{j=1}^p \langle \mathcal{A}_{\varphi_*,j} z_j, z_j \rangle - \lambda_{*,j} (z_j, z_j)_{L^2(\Omega)} \\ &= \sum_{j=1}^p \sum_{\ell \geq 2} \lambda_{\ell}(\mathcal{A}_{\varphi_*,j}) (\alpha_{j,\ell} v_{j,\ell}, z_j)_{L^2(\Omega)} - \lambda_1(\mathcal{A}_{\varphi_*,j}) (z_j, z_j)_{L^2(\Omega)} \\ &\geq \sum_{j=1}^p (\lambda_2(\mathcal{A}_{\varphi_*,j}) - \lambda_1(\mathcal{A}_{\varphi_*,j})) (z_j, z_j)_{L^2(\Omega)} > 0. \quad \square \end{aligned}$$

It immediately follows from the proof of Theorem 3.5 that $D_{\varphi\varphi}^2 \mathcal{L}(\varphi_*, \Lambda_*)$ is coercive on the tangent space of the constraint set with the coercivity constant $\gamma = \min_{j=1, \dots, p} (\lambda_2(\mathcal{A}_{\varphi_*,j}) - \lambda_1(\mathcal{A}_{\varphi_*,j})) > 0$.

4. GENERALISED OBLIQUE MANIFOLD

The ground state problem of multicomponent BECs is naturally connected to the infinite-dimensional generalised oblique manifold $\mathcal{OB}_N(p, H)$ defined in (2.2). In the finite-dimensional case, such a manifold with $N = I_p$ has been investigated in [1, 21, 55] in the context of the approximate joint diagonalisation problem, which frequently arises in data science and engineering. Here, we extend the results on the manifold geometry from these works to the infinite-dimensional setting.

First of all, note that $\mathcal{OB}_N(p, H)$ can be represented as the product manifold

$$(4.1) \quad \mathcal{OB}_N(p, H) = \mathcal{S}_{N_1} \times \dots \times \mathcal{S}_{N_p}$$

with the spheres $\mathcal{S}_{N_j} = \{\varphi \in H_0^1(\Omega) : \|\varphi\|_{L^2(\Omega)}^2 = N_j\}$ for $j = 1, \dots, p$. The geometric structure of \mathcal{S}_{N_j} , which is a particular case of the infinite-dimensional Stiefel manifold, has been studied in [8].

4.1. Tangent and normal spaces. The generalised oblique manifold $\mathcal{OB}_N(p, H)$ admits a submanifold structure on the ambient space H .

Proposition 4.1. *The generalised oblique manifold $\mathcal{OB}_N(p, H)$ is a closed embedded submanifold of the Hilbert space H of co-dimension p .*

Proof. We consider the map $F: H \rightarrow \mathcal{D}(p)$ given by

$$F(\varphi) = \langle\langle \varphi, \varphi \rangle\rangle - N.$$

Then it holds $\mathcal{OB}_N(p, H) = F^{-1}(0_p)$. This implies that $\mathcal{OB}_N(p, H)$ is closed, since it is the pre-image of the closed set $\{0_p\}$ for the continuous map F . We now show that F is a submersion or, equivalently, that for all $\varphi \in \mathcal{OB}_N(p, H)$, the Fréchet derivative of F at φ given by $DF(\varphi)[v] = 2 \langle\langle \varphi, v \rangle\rangle$ is surjective. Let $\Sigma \in \mathcal{D}(p)$. Then, for $v = \frac{1}{2}\varphi \Sigma N^{-1} \in H$, we obtain

$$DF(\varphi)[v] = \langle\langle \varphi, \varphi \Sigma N^{-1} \rangle\rangle = \Sigma.$$

Thus, by the submersion theorem [2, Prop. 3.3.3], $\mathcal{OB}_N(p, H)$ is an embedded submanifold of H and its co-dimension coincides with $\dim(\mathcal{D}(p)) = p$. \square

The kernel of $DF(\varphi)$ defines the *tangent space* $T_\varphi \mathcal{OB}_N(p, H)$ to $\mathcal{OB}_N(p, H)$ at φ . It is given by

$$T_\varphi \mathcal{OB}_N(p, H) = \ker(DF(\varphi)) = \{z \in H : \langle\langle \varphi, z \rangle\rangle = 0_p\}.$$

In order to introduce a Riemannian metric on $\mathcal{OB}_N(p, H)$, we consider a symmetric, bounded, and coercive bilinear form $g_\varphi: H \times H \rightarrow \mathbb{R}$ which defines an inner product on H . Further, let $\mathcal{G}_\varphi: H \rightarrow H^*$ be the linear bounded operator given by

$$\langle \mathcal{G}_\varphi v, w \rangle = g_\varphi(v, w) \quad \text{for all } v, w \in H.$$

Due to the coercivity of g_φ , there exists the inverse $\mathcal{G}_\varphi^{-1}: H^* \rightarrow H$ of \mathcal{G}_φ , which is also linear.

Since the generalised oblique manifold $\mathcal{OB}_N(p, H)$ is an embedded submanifold of H , the restriction $g_\varphi: T_\varphi \mathcal{OB}_N(p, H) \times T_\varphi \mathcal{OB}_N(p, H) \rightarrow \mathbb{R}$, provided that it depends smoothly on $\varphi \in H$, defines a Riemannian metric on $\mathcal{OB}_N(p, H)$ which turns $\mathcal{OB}_N(p, H)$ into a Riemannian manifold. Then the *normal space* to $\mathcal{OB}_N(p, H)$ at φ with respect to this metric is defined as

$$(T_\varphi \mathcal{OB}_N(p, H))_{g_\varphi}^\perp = \{\eta \in H : g_\varphi(\eta, z) = 0 \text{ for all } z \in T_\varphi \mathcal{OB}_N(p, H)\}.$$

Using the inverse operator \mathcal{G}_φ^{-1} , this space can be characterised as follows.

Proposition 4.2 (Characterisation of the normal space). *The normal space to $\mathcal{OB}_N(p, H)$ at $\varphi \in \mathcal{OB}_N(p, H)$ with respect to the metric g_φ is given by*

$$(T_\varphi \mathcal{OB}_N(p, H))_{g_\varphi}^\perp = \{\mathcal{G}_\varphi^{-1}(\varphi \Sigma) \in H : \Sigma \in \mathcal{D}(p)\}.$$

Proof. For all $z \in T_\varphi \mathcal{OB}_N(p, H)$ and $\Sigma \in \mathcal{D}(p)$, we see that

$$g_\varphi(\mathcal{G}_\varphi^{-1}(\varphi \Sigma), z) = (\varphi \Sigma, z)_L = \text{trace} \langle\langle \varphi \Sigma, z \rangle\rangle = \text{trace} (\Sigma \langle\langle \varphi, z \rangle\rangle) = 0.$$

This implies that $\{\mathcal{G}_\varphi^{-1}(\varphi \Sigma) \in H : \Sigma \in \mathcal{D}(p)\} \subseteq (T_\varphi \mathcal{OB}_N(p, H))_{g_\varphi}^\perp$. The equality follows since both spaces have dimension p . \square

The orthogonal projection $\mathcal{P}_\varphi: H \rightarrow T_\varphi \mathcal{OB}_N(p, H)$ with respect to the metric g_φ will be called the *g_φ -orthogonal projection* and is characterised in terms of the inverse operator below.

Proposition 4.3. *Let $\varphi \in \mathcal{OB}_N(p, H)$. Then the g_φ -orthogonal projection onto the tangent space $T_\varphi \mathcal{OB}_N(p, H)$ is given by*

$$(4.2) \quad \mathcal{P}_\varphi(\mathbf{u}) = \mathbf{u} - \mathcal{G}_\varphi^{-1}(\varphi \Sigma_{\varphi, \mathbf{u}}), \quad \mathbf{u} \in H,$$

where $\Sigma_{\varphi, \mathbf{u}} \in \mathcal{D}(p)$ is the unique solution to the equation

$$(4.3) \quad \langle\langle \varphi, \mathcal{G}_\varphi^{-1}(\varphi \Sigma_{\varphi, \mathbf{u}}) \rangle\rangle = \langle\langle \varphi, \mathbf{u} \rangle\rangle.$$

Proof. First, we show that equation (4.3) is uniquely solvable and provide its explicit solution. Let $\varphi \in \mathcal{OB}_N(p, H)$ and $\Sigma_{\varphi, \mathbf{u}} = \text{diag}(\sigma_1, \dots, \sigma_p)$. For every component φ_j of φ , we define the p -frame $\hat{\varphi}_j = (0, \dots, 0, \varphi_j, 0, \dots, 0)$ for $j = 1, \dots, p$. Then, due to the linearity of \mathcal{G}_φ^{-1} , we obtain that $\mathcal{G}_\varphi^{-1}(\varphi \Sigma_{\varphi, \mathbf{u}}) = \sum_{i=1}^p \sigma_i \mathcal{G}_\varphi^{-1} \hat{\varphi}_i$. In this case, equation (4.3) can equivalently be written as a linear system $\hat{G}\sigma = \hat{u}$ with an unknown vector $\sigma = [\sigma_1, \dots, \sigma_p]^T$ and given

$$(4.4) \quad \hat{G} = \begin{bmatrix} (\varphi_1, (\mathcal{G}_\varphi^{-1} \hat{\varphi}_1)_1)_{L^2(\Omega)} & \cdots & (\varphi_1, (\mathcal{G}_\varphi^{-1} \hat{\varphi}_p)_1)_{L^2(\Omega)} \\ \vdots & \ddots & \vdots \\ (\varphi_p, (\mathcal{G}_\varphi^{-1} \hat{\varphi}_1)_p)_{L^2(\Omega)} & \cdots & (\varphi_p, (\mathcal{G}_\varphi^{-1} \hat{\varphi}_p)_p)_{L^2(\Omega)} \end{bmatrix}, \quad \hat{u} = \begin{bmatrix} (\varphi_1, u_1)_{L^2(\Omega)} \\ \vdots \\ (\varphi_p, u_p)_{L^2(\Omega)} \end{bmatrix}.$$

We now verify that the matrix \hat{G} is nonsingular. Assume that there exists a vector $\alpha = [\alpha_1, \dots, \alpha_p]^T$ such that $\hat{G}\alpha = 0$. This implies that

$$(\varphi_i, (\mathcal{G}_\varphi^{-1}(\varphi \text{diag}(\alpha)))_i)_{L^2(\Omega)} = \sum_{j=1}^p \alpha_j (\varphi_i, (\mathcal{G}_\varphi^{-1} \hat{\varphi}_j)_i)_{L^2(\Omega)} = 0, \quad i = 1, \dots, p,$$

and, hence, $\mathcal{G}_\varphi^{-1}(\varphi \text{diag}(\alpha)) \in T_\varphi \mathcal{OB}_N(p, H)$. On the other hand, due to Proposition 4.2, we have $\mathcal{G}_\varphi^{-1}(\varphi \text{diag}(\alpha)) \in (T_\varphi \mathcal{OB}_N(p, H))_{g_\varphi}^\perp$ and thus $\mathcal{G}_\varphi^{-1}(\varphi \text{diag}(\alpha)) = \mathbf{0}$. This yields that $\alpha = 0$ which implies that \hat{G} is nonsingular and $\Sigma_{\varphi, \mathbf{u}} = \text{diag}(\sigma) = \text{diag}(\hat{G}^{-1} \hat{u})$ is the unique solution of (4.3).

Next, we prove that \mathcal{P}_φ maps on $T_\varphi \mathcal{OB}_N(p, H)$. Indeed, it follows from (4.3) that

$$\langle\langle \varphi, \mathcal{P}_\varphi(\mathbf{u}) \rangle\rangle = \langle\langle \varphi, \mathbf{u} - \mathcal{G}_\varphi^{-1}(\varphi \Sigma_{\varphi, \mathbf{u}}) \rangle\rangle = 0$$

and, hence, $\mathcal{P}_\varphi(\mathbf{u}) \in T_\varphi \mathcal{OB}_N(p, H)$ for all $\mathbf{u} \in H$.

Further, taking into account that for all $\mathbf{u} \in T_\varphi \mathcal{OB}_N(p, H)$, equation (4.3) has only the trivial solution $\Sigma_{\varphi, \mathbf{u}} = 0_p$, we obtain that

$$\mathcal{P}_\varphi(\mathcal{P}_\varphi(\mathbf{u})) = \mathcal{P}_\varphi(\mathbf{u}) - \mathcal{G}_\varphi^{-1}(\varphi \Sigma_{\varphi, \mathcal{P}_\varphi(\mathbf{u})}) = \mathcal{P}_\varphi(\mathbf{u}).$$

This shows that \mathcal{P}_φ is a projection. Finally, it follows from Proposition 4.2 that

$$\mathbf{u} - \mathcal{P}_\varphi(\mathbf{u}) = \mathcal{G}_\varphi^{-1}(\varphi \Sigma_{\varphi, \mathbf{u}}) \in (T_\varphi \mathcal{OB}_N(p, H))_{g_\varphi}^\perp$$

implying the g_φ -orthogonality property. \square

The computation of the projection \mathcal{P}_φ in (4.2) requires multiple inversions of the operator \mathcal{G}_φ , which can be computationally expensive in practice. To reduce the computational cost, we exploit the product structure of the generalised oblique manifold in (4.1) and, inspired by [35], equip it with a Riemannian metric defined as a sum of the metrics $g_{\varphi, j}$ on each component \mathcal{S}_{N_j} , i.e.,

$$(4.5) \quad g_\varphi^\times(\mathbf{z}, \mathbf{y}) = g_{\varphi, 1}(z_1, y_1) + \dots + g_{\varphi, p}(z_p, y_p)$$

for $\mathbf{z} = (z_1, \dots, z_p)$, $\mathbf{y} = (y_1, \dots, y_p) \in T_\varphi \mathcal{OB}_N(p, H)$. Here,

$$g_{\varphi, j}(z_j, y_j) = \langle \mathcal{G}_{\varphi, j}^\times y_j, z_j \rangle \quad \text{for all } z_j, y_j \in T_{\varphi_j} \mathcal{S}_{N_j}$$

with appropriate operators $\mathcal{G}_{\varphi, j}^\times: H_0^1(\Omega) \rightarrow H^{-1}(\Omega)$, $j = 1, \dots, p$, smoothly depending on $\varphi \in H$. The metric g_φ^\times has an advantage over g_φ in that all computations can be performed component-wise, which facilitates parallel computing. As a consequence of Proposition 4.3, by exploiting the additive structure of the metric g_φ^\times in (4.5), we obtain the following representation for the g_φ^\times -orthogonal projection onto $T_\varphi \mathcal{OB}_N(p, H)$.

Corollary 4.4. *Define the operator $\mathcal{G}_\varphi^\times \mathbf{v} = (\mathcal{G}_{\varphi, 1}^\times v_1, \dots, \mathcal{G}_{\varphi, p}^\times v_p)$ for $\mathbf{v} \in H$. Then the g_φ^\times -orthogonal projection onto $T_\varphi(\mathcal{OB}_N(p, H))$ is given by $\mathcal{P}_\varphi^\times(\mathbf{u}) = \mathbf{u} - (\mathcal{G}_\varphi^\times)^{-1} \varphi \Sigma_{\varphi, \mathbf{u}}^\times$ with the diagonal matrix $\Sigma_{\varphi, \mathbf{u}}^\times = \langle\langle \varphi, (\mathcal{G}_\varphi^\times)^{-1} \varphi \rangle\rangle^{-1} \langle\langle \varphi, \mathbf{u} \rangle\rangle$.*

Proof. The result follows from Proposition 4.3 by using the fact that for the metric g_φ^\times in (4.5), the matrix \hat{G} given in (4.4) is diagonal with entries $(\varphi_j, (\mathcal{G}_{\varphi,j}^\times)^{-1}\varphi_j)_{L^2(\Omega)}$ on the diagonal. \square

4.2. Riemannian gradients and Hessians. The *Riemannian gradient* of a Fréchet differentiable functional \mathcal{E} defined on $\mathcal{OB}_N(p, H)$ with respect to the metric g_φ is the unique element $\text{grad } \mathcal{E}(\varphi)$ in the tangent space $T_\varphi \mathcal{OB}_N(p, H)$ which satisfies the condition

$$g_\varphi(\text{grad } \mathcal{E}(\varphi), z) = \text{D } \mathcal{E}(\varphi)[z] \quad \text{for all } z \in T_\varphi \mathcal{OB}_N(p, H).$$

The Riemannian gradient of the energy functional \mathcal{E} in (1.2) with respect to g_φ can be represented as

$$(4.6) \quad \text{grad } \mathcal{E}(\varphi) = \mathcal{P}_\varphi(\mathcal{G}_\varphi^{-1} \text{D } \mathcal{E}(\varphi)) = \mathcal{G}_\varphi^{-1} \mathcal{A}_\varphi \varphi - \mathcal{G}_\varphi^{-1}(\varphi \Sigma_{\varphi, \mathcal{G}_\varphi^{-1} \mathcal{A}_\varphi \varphi}),$$

where $\Sigma_{\varphi, \mathcal{G}_\varphi^{-1} \mathcal{A}_\varphi \varphi}$ is as in Proposition 4.3 with $\mathbf{u} = \mathcal{G}_\varphi^{-1} \mathcal{A}_\varphi \varphi$.

Consider the linear operator $\mathcal{R}_\varphi: H \rightarrow H^*$ defined by $\mathcal{R}_\varphi \mathbf{v} = \mathcal{A}_\varphi \mathbf{v} - \varphi \langle \varphi, \mathcal{A}_\varphi \mathbf{v} \rangle N^{-1}$. Just as \mathcal{A}_φ , the operator \mathcal{R}_φ acts component-wise with the component operators denoted by $\mathcal{R}_{\varphi,j}$. For all $\mathbf{v} \in H$ with $\mathcal{A}_\varphi \mathbf{v} \in H$, we have $\langle \varphi, \mathcal{R}_\varphi \mathbf{v} \rangle = 0$ implying that $\mathcal{R}_\varphi \mathbf{v} \in T_\varphi \mathcal{OB}_N(p, H)$. Note that $\mathcal{R}_\varphi \varphi$ gives the residual of the NLEVP (3.2). It can also be used to obtain an alternative representation for the Riemannian gradient, namely

$$\text{grad } \mathcal{E}(\varphi) = \mathcal{P}_\varphi(\mathcal{G}_\varphi^{-1} \mathcal{R}_\varphi \varphi) = \mathcal{G}_\varphi^{-1} \mathcal{R}_\varphi \varphi - \mathcal{G}_\varphi^{-1}(\varphi \Sigma_{\varphi, \mathcal{G}_\varphi^{-1} \mathcal{R}_\varphi \varphi}),$$

where $\Sigma_{\varphi, \mathcal{G}_\varphi^{-1} \mathcal{R}_\varphi \varphi}$ is as in Proposition 4.3 with $\mathbf{u} = \mathcal{G}_\varphi^{-1} \mathcal{R}_\varphi \varphi$.

Let the Riemannian manifold $(\mathcal{OB}_N(p, H), g_\varphi)$ be endowed with the Riemannian connection ∇ . The *Riemannian Hessian* of a twice differentiable functional \mathcal{E} , denoted by $\text{Hess } \mathcal{E}(\varphi)$, is the linear mapping $\text{Hess } \mathcal{E}(\varphi): T_\varphi \mathcal{OB}_N(p, H) \rightarrow T_\varphi \mathcal{OB}_N(p, H)$ given by

$$\text{Hess } \mathcal{E}(\varphi)[z] = \nabla_z \text{grad } \mathcal{E}(\varphi) \quad \text{for all } z \in T_\varphi \mathcal{OB}_N(p, H),$$

where ∇_z denotes the covariant derivative along z with respect to the connection ∇ . If the metric does not depend on φ , the Riemannian Hessian admits the expression

$$(4.7) \quad \text{Hess } \mathcal{E}(\varphi)[z] = \mathcal{P}_\varphi(\text{D grad } \mathcal{E}(\varphi)[z]),$$

which can be shown similarly to the finite-dimensional case [2, Prop. 5.3.2].

4.3. Choices of metric. We introduce several metrics on the manifold $\mathcal{OB}_N(p, H)$ and discuss the corresponding geometric concepts. In particular, using first- and second-order information of the energy, we construct specific metrics that possess a preconditioning effect when used in Riemannian optimisation.

4.3.1. L^2 -metric. Let $\mathcal{G}_L: H \rightarrow H^*$ denote the canonical identification operator defined by

$$\langle \mathcal{G}_L \mathbf{v}, \mathbf{w} \rangle = (\mathbf{v}, \mathbf{w})_L \quad \text{for all } \mathbf{v}, \mathbf{w} \in H.$$

This allows us to equip the generalised oblique manifold $\mathcal{OB}_N(p, H)$ with the L^2 -metric

$$(4.8) \quad g_L(\mathbf{z}, \mathbf{y}) = \langle \mathcal{G}_L \mathbf{z}, \mathbf{y} \rangle, \quad \mathbf{z}, \mathbf{y} \in T_\varphi \mathcal{OB}_N(p, H),$$

which is independent of φ . Note that this metric violates our assumptions above, as it is not coercive with respect to the H -norm. As a consequence, the operator \mathcal{G}_L is not necessarily invertible and the Riemannian gradient with respect to g_L may not exist for all φ . In this subsection, however, we will always assume that all formulas are well-defined and, in particular, that $\varphi \in H$ is such that $\mathcal{A}_\varphi \varphi \in H$.

As the metric g_L is of the additive form (4.5), the L^2 -orthogonal projection onto $T_\varphi \mathcal{OB}_N(p, H)$ reads

$$(4.9) \quad \mathcal{P}_{\varphi,L}(\mathbf{u}) = \mathbf{u} - \varphi \langle \varphi, \mathbf{u} \rangle N^{-1}, \quad \mathbf{u} \in H.$$

The Riemannian gradient of \mathcal{E} in (1.2) with respect to g_L then takes the form

$$(4.10) \quad \text{grad}_L \mathcal{E}(\varphi) = \mathcal{P}_{\varphi,L}(\text{D } \mathcal{E}(\varphi)) = \mathcal{A}_\varphi \varphi - \varphi \langle \varphi, \mathcal{A}_\varphi \varphi \rangle N^{-1} = \mathcal{R}_\varphi \varphi.$$

Furthermore, using (3.4), we obtain from (4.7) the Riemannian Hessian

$$(4.11) \quad \begin{aligned} \text{Hess}_L \mathcal{E}(\varphi)[z] &= \mathcal{P}_{\varphi,L}(\mathcal{A}_\varphi z + \mathcal{B}_\varphi(z, \varphi) - z \langle \varphi, \mathcal{A}_\varphi \varphi \rangle N^{-1}) \\ &= \mathcal{A}_\varphi z + \mathcal{B}_\varphi(z, \varphi) - \varphi \langle \varphi, \mathcal{A}_\varphi z + \mathcal{B}_\varphi(z, \varphi) \rangle N^{-1} - z \langle \varphi, \mathcal{A}_\varphi \varphi \rangle N^{-1}. \end{aligned}$$

Note that for a constrained critical point $\varphi^* \in \mathcal{OB}_N(p, H)$ of \mathcal{E} and the corresponding Lagrange multiplier Λ^* , the Riemannian Hessian of \mathcal{E} and the second-order derivative of the Lagrange functional \mathcal{L} are related to each other via $\text{Hess}_L \mathcal{E}(\varphi^*)[z] = \mathcal{P}_{\varphi^*, L}(\text{D}_{\varphi\varphi}^2 \mathcal{L}(\varphi^*, \Lambda^*)[z])$ for all tangent vectors $z \in T_{\varphi^*} \mathcal{OB}_N(p, H)$. Moreover, it follows from Theorem 3.5 that for a ground state φ_* , the Riemannian Hessian $\text{Hess}_L \mathcal{E}(\varphi_*)$ is positive definite on the tangent space $T_{\varphi_*} \mathcal{OB}_N(p, H)$.

4.3.2. Energy-adaptive metric. By using the inner product $a_\varphi(\cdot, \cdot)$ introduced in (2.7), we define an alternative Riemannian metric on the manifold $\mathcal{OB}_N(p, H)$, namely

$$(4.12) \quad g_{\varphi, a}(z, \mathbf{y}) = a_\varphi(z, \mathbf{y}) \quad \text{for all } z, \mathbf{y} \in T_\varphi \mathcal{OB}_N(p, H).$$

It is referred to as the *energy-adaptive metric*. As discussed in the wake of Proposition 2.2, coercivity of a_φ can, in general, be achieved only by a shift in the potential with a constant C_φ depending on φ . For the iterative optimisation method presented in Section 5.1.2, we will show in Section 6.1 that such a shift can be chosen relying on the initial guess only.

It follows from Corollary 4.4 with $\mathcal{G}_\varphi^\times = \mathcal{A}_\varphi$, which obviously acts component-wise, that the *a_φ -orthogonal projection* onto the tangent space $T_\varphi \mathcal{OB}_N(p, H)$ is given by

$$\mathcal{P}_{\varphi, a}(\mathbf{u}) = \mathbf{u} - \mathcal{A}_\varphi^{-1} \varphi \langle \varphi, \mathbf{u} \rangle \langle \varphi, \mathcal{A}_\varphi^{-1} \varphi \rangle^{-1}.$$

Furthermore, using (4.6), the Riemannian gradient of \mathcal{E} in (1.2) with respect to the energy-adaptive metric $g_{\varphi, a}$ is determined as

$$(4.13) \quad \text{grad}_a \mathcal{E}(\varphi) = \mathcal{P}_{\varphi, a}(\varphi) = \varphi - \mathcal{A}_\varphi^{-1} \varphi N \langle \varphi, \mathcal{A}_\varphi^{-1} \varphi \rangle^{-1} = \mathcal{P}_{\varphi, a}(\mathcal{A}_\varphi^{-1} \mathcal{R}_\varphi \varphi).$$

Using the relation $\mathcal{A}_\varphi^{-1} \varphi = (\varphi - \mathcal{A}_\varphi^{-1} \mathcal{R}_\varphi \varphi) \langle \varphi, \mathcal{A}_\varphi \varphi \rangle^{-1} N$, which follows directly from the definition of $\mathcal{R}_\varphi \varphi$, it can further be represented as

$$(4.14) \quad \text{grad}_a \mathcal{E}(\varphi) = \varphi - (\varphi - \mathcal{A}_\varphi^{-1} \mathcal{R}_\varphi \varphi) (I_p - N^{-1} \langle \varphi, \mathcal{A}_\varphi^{-1} \mathcal{R}_\varphi \varphi \rangle)^{-1}.$$

The Riemannian Hessian with respect to $g_{\varphi, a}$ can be calculated with the help of [51, Th. 3.1]. This, however, is beyond the scope of the present paper.

4.3.3. Lagrangian-based metric. In [46, 50, 56], different strategies for constructing Riemannian metrics have been proposed in the context of Riemannian preconditioning for solving various optimisation problems on matrix manifolds. They all aim to speed up the convergence of Riemannian optimisation methods by exploiting the second-order information of the cost functional and possibly constraints. Here, we adapt the approaches from [50] and [35] to the infinite-dimensional setting with product manifold structure and develop a new family of Riemannian metrics by considering the second-order derivative of a regularised Lagrange functional and neglecting its off-diagonal blocks with a goal to trade-off between the computational cost and efficiency.

Let us start with introducing a regularised Lagrange functional

$$\mathcal{L}_\omega(\varphi, \Lambda) = \mathcal{E}(\varphi) - \frac{\omega}{2} \text{trace} \left(\Lambda (\langle \varphi, \varphi \rangle - N) \right)$$

with an appropriately chosen regularisation parameter $\omega \geq 0$. Note that for $\omega = 1$, \mathcal{L}_ω coincides with the Lagrangian \mathcal{L} in (3.1). The second-order derivative of \mathcal{L}_ω with respect to φ has the form

$$(4.15) \quad \text{D}_{\varphi\varphi}^2 \mathcal{L}_\omega(\varphi, \Lambda)[\mathbf{v}] = \mathcal{A}_\varphi \mathbf{v} + \mathcal{B}_\varphi(\mathbf{v}, \varphi) - \omega \mathbf{v} \Lambda$$

with \mathcal{A}_φ and \mathcal{B}_φ given in (2.10) and (3.5), respectively. We define now an operator $\mathcal{G}_{\varphi, \omega}: H \rightarrow H^*$ acting component-wise, i.e., $\mathcal{G}_{\varphi, \omega} \mathbf{v} = (\mathcal{G}_{\varphi, \omega, 1} v_1, \dots, \mathcal{G}_{\varphi, \omega, p} v_p)$, where

$$\mathcal{G}_{\varphi, \omega, j} v_j = \mathcal{A}_{\varphi, j} v_j + \mathcal{B}_{\varphi, jj}(v_j, \varphi_j) - \omega \lambda_j v_j, \quad j = 1, \dots, p,$$

are obtained from (4.15) by neglecting $\mathcal{B}_{\varphi, ij}$ with $i \neq j$ and setting the diagonal elements of Λ to $\lambda_j = \langle \mathcal{A}_{\varphi, j} \varphi_j, \varphi_j \rangle / N_j$, $j = 1, \dots, p$. Since $a_\varphi(\cdot, \cdot)$ is assumed to be coercive and for all $v_j \in H_0^1(\Omega)$ it holds that $\langle \mathcal{B}_{\varphi, jj}(v_j, \varphi_j), v_j \rangle \geq 0$, choosing the parameter ω sufficiently small guarantees that the bilinear form $g_{\varphi, \omega}(\mathbf{v}, \mathbf{w}) = \langle \mathcal{G}_{\varphi, \omega} \mathbf{v}, \mathbf{w} \rangle$ is coercive. This allows us to define a new metric on the generalised oblique manifold $\mathcal{OB}_N(p, H)$ via

$$(4.16) \quad g_{\varphi, \omega}(z, \mathbf{y}) = \langle \mathcal{G}_{\varphi, \omega} z, \mathbf{y} \rangle = \sum_{j=1}^p \langle \mathcal{G}_{\varphi, \omega, j} z_j, y_j \rangle \quad \text{for all } z, \mathbf{y} \in T_\varphi \mathcal{OB}_N(p, H).$$

Due to the additive structure of this metric, the corresponding Riemannian gradient of the energy functional \mathcal{E} is given by

$$\text{grad}_\omega \mathcal{E}(\varphi) = \mathcal{G}_{\varphi,\omega}^{-1} \mathcal{R}_\varphi \varphi - \mathcal{G}_{\varphi,\omega}^{-1} \varphi \langle\langle \varphi, \mathcal{G}_{\varphi,\omega}^{-1} \mathcal{R}_\varphi \varphi \rangle\rangle \langle\langle \varphi, \mathcal{G}_{\varphi,\omega}^{-1} \varphi \rangle\rangle^{-1}.$$

In summary, we see that different metrics result in distinct Riemannian gradients. The choice of the metric, as we will see in what follows, significantly influences the performance of the Riemannian optimisation schemes. A carefully chosen metric enables efficient optimisation by ensuring that the geometry of the generalised oblique manifold $\mathcal{OB}_N(p, H)$ is respected in every optimisation step.

5. RIEMANNIAN OPTIMISATION METHODS

This section presents several Riemannian optimisation schemes for solving the energy minimisation problem (2.3). To facilitate this, we need a retraction, which allows movement in a tangent direction while remaining on the manifold. This can be realised by using a component-wise normalisation operator $\mathcal{N}: H \rightarrow \mathcal{OB}_N(p, H)$ defined as

$$(5.1) \quad \mathcal{N}(\mathbf{v}) = \mathbf{v} \langle\langle \mathbf{v}, \mathbf{v} \rangle\rangle^{-1/2} N^{1/2}, \quad \mathbf{v} \in H.$$

Clearly, for all $\varphi \in \mathcal{OB}_N(p, H)$ and $\mathbf{z} \in T_\varphi \mathcal{OB}_N(p, H)$, $\mathcal{N}(\varphi + \mathbf{z})$ is well-defined, as the matrix $\langle\langle \varphi + \mathbf{z}, \varphi + \mathbf{z} \rangle\rangle = N + \langle\langle \mathbf{z}, \mathbf{z} \rangle\rangle$ is invertible. Moreover, for the origin $\mathbf{0}_\varphi \in T_\varphi \mathcal{OB}_N(p, H)$, we have $\mathcal{N}(\varphi + \mathbf{0}_\varphi) = \varphi$, and for all $\mathbf{z} \in T_\varphi \mathcal{OB}_N(p, H)$, the local rigidity condition $\left. \frac{d}{dt} \mathcal{N}(\varphi + t\mathbf{z}) \right|_{t=0} = \mathbf{z}$ is satisfied. This shows that the mapping $(\varphi, \mathbf{z}) \mapsto \mathcal{N}(\varphi + \mathbf{z})$ on the tangent bundle of $\mathcal{OB}_N(p, H)$ indeed defines a retraction on this manifold.

5.1. Preconditioned Riemannian gradient descent methods. A simple first-order optimisation scheme is the gradient descent method. In the context of Riemannian optimisation, this iterative procedure consists of the following steps: move in the tangent space along a descent direction given by the negative Riemannian gradient with a certain step size and then retract the resulting tangent vector back onto the manifold. In a general setting, the *Riemannian gradient descent (RGD) method* is described in Algorithm 1.

Algorithm 1 Riemannian gradient descent method

Require: Metric g_φ on $\mathcal{OB}_N(p, H)$, initial guess $\varphi_0 \in \mathcal{OB}_N(p, H)$.

for $k = 0, 1, \dots$ **do**
 Compute a search direction $\mathbf{z}_k = -\text{grad } \mathcal{E}(\varphi_k)$.
 Choose a step size $\tau_k > 0$.
 Update $\varphi_{k+1} = \mathcal{N}(\varphi_k + \tau_k \mathbf{z}_k)$.
end for

The convergence of the RGD method is strongly influenced by the step size, which can be adaptively determined using, e.g., the non-monotone line search procedure combined with the alternating Barzilai–Borwein step size strategy [59, 61]. It should also be noted that the RGD method depends on the choice of retraction and, most importantly, on the selected metric. In what follows, we briefly describe the resulting RGD schemes for the energy minimisation problem (2.3) based on the metrics considered in Section 4.3 and highlight relationships between them.

5.1.1. Preconditioned L^2 -Riemannian gradient descent method. The choice of the L^2 -metric g_L defined in (4.8) in Algorithm 1 yields the L^2 -RGD method which can be interpreted as a power iteration with shifting. In electronic structure calculations, this method is also known as the direct minimisation algorithm [52, 54]. However, due to its explicit nature, it generally requires preconditioning which leads to the iteration

$$\varphi_{k+1} = \mathcal{N}\left(\varphi_k - \tau_k \mathcal{P}_{\varphi_k, L}(\mathcal{C}_{\varphi_k}^{-1}(\mathcal{A}_{\varphi_k} \varphi_k - \varphi_k \langle\langle \varphi_k, \mathcal{A}_{\varphi_k} \varphi_k \rangle\rangle N^{-1}))\right)$$

with a preconditioner \mathcal{C}_{φ_k} . Formally, this scheme requires a sufficiently smooth starting value to be well-defined. Different physics-based preconditioners related to the Laplace and Thomas–Fermi approximations have been developed in the literature [11, 12]. Alternatively, following [8], we

propose the preconditioner $\mathcal{C}_{\varphi_k} = \mathcal{A}_{\varphi_k}$. Then using expression (4.9), we obtain the *energy-preconditioned L^2 -RGD method*

$$(5.2) \quad \varphi_{k+1} = \mathcal{N}\left(\varphi_k - \tau_k \left(\varphi_k - \mathcal{A}_{\varphi_k}^{-1} \varphi_k N \langle\langle \varphi_k, \mathcal{A}_{\varphi_k}^{-1} \varphi_k \rangle\rangle^{-1}\right) \Theta_{\varphi_k}\right)$$

with the diagonal matrix $\Theta_{\varphi_k} = N^{-1} \langle\langle \varphi_k, \mathcal{A}_{\varphi_k}^{-1} \varphi_k \rangle\rangle \langle\langle \varphi_k, \mathcal{A}_{\varphi_k} \varphi_k \rangle\rangle N^{-1}$.

5.1.2. Energy-adaptive Riemannian gradient descent method. Endowing $\mathcal{OB}_N(p, H)$ with the energy-adaptive metric $g_{\varphi, a}$ defined in (4.12) and using (4.13) and (4.14), we obtain the *energy-adaptive Riemannian gradient descent (eaRGD) method*

$$(5.3) \quad \varphi_{k+1} = \mathcal{N}\left(\varphi_k - \tau_k \left(\varphi_k - \mathcal{A}_{\varphi_k}^{-1} \varphi_k N \langle\langle \varphi_k, \mathcal{A}_{\varphi_k}^{-1} \varphi_k \rangle\rangle^{-1}\right)\right)$$

$$(5.4) \quad = \mathcal{N}\left(\varphi_k - \tau_k \left(\varphi_k - \left(\varphi_k - \mathcal{A}_{\varphi_k}^{-1} \mathcal{R}_{\varphi_k} \varphi_k\right) \left(I_p - N^{-1} \langle\langle \varphi_k, \mathcal{A}_{\varphi_k}^{-1} \mathcal{R}_{\varphi_k} \varphi_k \rangle\rangle\right)^{-1}\right)\right).$$

This method can be interpreted as the inverse subspace iteration for \mathcal{A}_{φ} enhanced with adaptive damping, where τ_k represents the damping parameter; see [38, 41] for the case $p = 1$. For $\tau_k = 1$, it reduces to the inverse subspace iteration method, known also as the \mathcal{A} -method. Very similar schemes, such as the discrete normalised gradient flows [19], result from an implicit–explicit time discretisation of the continuous L^2 -Riemannian gradient flow; see also [30, 39].

The eaRGD method (5.3) differs from the particular preconditioned L^2 -RGD iteration (5.2) only by the diagonal matrix Θ_{φ_k} . Since at a critical point, $\mathcal{A}_{\varphi} \varphi = \varphi \Lambda$ and $\mathcal{A}_{\varphi}^{-1} \varphi = \varphi \Lambda^{-1}$, the RGD methods (5.2) and (5.3) are even asymptotically equivalent. In numerical experiments in Section 8, we implement (5.4), as it explicitly includes the residual $\mathcal{R}_{\varphi_k} \varphi_k$.

5.1.3. Lagrangian-based Riemannian gradient descent method. By considering the Lagrangian-based metric $g_{\varphi, \omega}$ as defined in (4.16), we derive the *Lagrangian-based Riemannian gradient descent (LgrRGD) method*

$$(5.5) \quad \varphi_{k+1} = \mathcal{N}\left(\varphi_k - \tau_k \left(\mathcal{G}_{\varphi_k, \omega_k}^{-1} \mathcal{R}_{\varphi_k} \varphi_k - \mathcal{G}_{\varphi_k, \omega_k}^{-1} \varphi_k \Sigma_{\varphi_k, \omega_k}\right)\right)$$

with the diagonal matrix $\Sigma_{\varphi_k, \omega_k} = \langle\langle \varphi_k, \mathcal{G}_{\varphi_k, \omega_k}^{-1} \mathcal{R}_{\varphi_k} \varphi_k \rangle\rangle \langle\langle \varphi_k, \mathcal{G}_{\varphi_k, \omega_k}^{-1} \varphi_k \rangle\rangle^{-1}$ and the regularisation parameter $\omega_k \in (0, 1]$ guaranteeing that $\mathcal{G}_{\varphi_k, \omega_k}$ is invertible. A possible choice for ω_k can be found in [50]. In practice, however, we observed that after initialising the algorithm sufficiently close to a ground state (e.g. by applying a few steps of eaRGD first), simply choosing $\omega_k = 1$ usually works well. Comparing the computational complexity of the eaRGD method (5.4) and the LgrRGD method (5.5), we see that each iteration of the latter requires the solution of two linear operator equations with the same operator $\mathcal{G}_{\varphi_k, \omega}$ and the right-hand sides $\mathcal{R}_{\varphi_k} \varphi_k$ and φ_k , while the former involves the solution of a single equation with the operator \mathcal{A}_{φ_k} and the right-hand side $\mathcal{R}_{\varphi_k} \varphi_k$.

5.2. Alternating Riemannian gradient descent method. In the above RGD schemes, the metric is of additive form (4.5), so that the components $\varphi_{k+1, j}$ of the new iteration φ_{k+1} can be calculated independently, giving rise to possible parallelisation. Alternatively, inspired by the alternating approach presented in [43], the components of the new iteration can be computed sequentially using the components most recently calculated. This leads to the *alternating RGD method* presented in Algorithm 2, which is formulated for a general metric g_{φ}^{\times} of the form (4.5) induced by an operator $\mathcal{G}_{\varphi}^{\times}$ acting component-wise. By taking either $\mathcal{G}_{\varphi}^{\times} = \mathcal{A}_{\varphi}$ or $\mathcal{G}_{\varphi}^{\times} = \mathcal{G}_{\varphi, \omega}$, we get the corresponding alternating versions of the eaRGD and LgrRGD methods, where for the eaRGD method, we can use (5.3) or (5.4) to reduce the number of linear systems to be solved per alternating step by one. The alternating LgrRGD method is similar to the alternating Newton–Noda method presented in [43], but with a different choice for the Lagrange multiplier.

5.3. Riemannian Newton and Newton-type methods. In the *Riemannian Newton (RN) method*, for given $\varphi_k \in \mathcal{OB}_N(p, H)$, the search direction $z_k \in T_{\varphi_k} \mathcal{OB}_N(p, H)$ is computed by solving the Newton equation

$$(5.6) \quad \text{Hess } \mathcal{E}(\varphi_k)[z_k] = -\text{grad } \mathcal{E}(\varphi_k),$$

leading to the next iterate $\varphi_{k+1} = \mathcal{N}(\varphi_k + z_k)$. The resulting method is given in Algorithm 3.

In the L^2 -metric, due to (4.10) and (4.11), the Newton equation (5.6) takes the form

$$(5.7) \quad \mathcal{P}_{\varphi_k, L}(\mathcal{A}_{\varphi_k} z_k + \mathcal{B}_{\varphi_k}(z_k, \varphi_k) - z_k \langle\langle \varphi_k, \mathcal{A}_{\varphi_k} \varphi_k \rangle\rangle N^{-1}) = -\mathcal{R}_{\varphi_k} \varphi_k.$$

Algorithm 2 Alternating Riemannian gradient descent method

Require: Operator $\mathcal{G}_\varphi^\times$ defining the metric g_φ^\times on $\mathcal{OB}_N(p, H)$, initial guess $\varphi_0 \in \mathcal{OB}_N(p, H)$.

```

for  $k = 0, 1, \dots$  do
  Set  $\varphi_{k+1} = \varphi_k$ .
  for  $j = 1, \dots, p$  do
    Solve  $\mathcal{G}_{\varphi_{k+1},j}^\times v = \mathcal{R}_{\varphi_{k+1},j} \varphi_{k,j}$  for  $v$ .
    Solve  $\mathcal{G}_{\varphi_{k+1},j}^\times w = \varphi_{k,j}$  for  $w$ .
    Compute  $z = v - \frac{(\varphi_{k,j},v)_{L^2(\Omega)}}{(\varphi_{k,j},w)_{L^2(\Omega)}} w$ .
    Choose a step size  $\tau_k > 0$ .
    Update  $\varphi_{k+1,j} = \sqrt{N_j} \frac{\varphi_{k,j} + \tau_k z}{\|\varphi_{k,j} + \tau_k z\|_{L^2(\Omega)}}$ .
  end for
end for

```

Algorithm 3 Riemannian Newton method

Require: Metric g_φ on $\mathcal{OB}_N(p, H)$, initial guess $\varphi_0 \in \mathcal{OB}_N(p, H)$.

```

for  $k = 0, 1, \dots$  do
  Solve Hess  $\mathcal{E}(\varphi_k)[z_k] = -\text{grad } \mathcal{E}(\varphi_k)$  for  $z_k \in T_{\varphi_k} \mathcal{OB}_N(p, H)$ .
  Update  $\varphi_{k+1} = \mathcal{N}(\varphi_k + z_k)$ .
end for

```

As in Section 5.1.1, it needs to hold $\mathcal{A}_{\varphi_k} \varphi_k \in H$. Similarly to [9], we can show that the resulting RN method is equivalent to the Lagrange–Newton method [3] and the Newton–Noda iteration [32] with modified update $\varphi_{k+1} = \mathcal{N}(\varphi_k + z_k)$ and $\Lambda_{k+1} = \langle\langle \varphi_{k+1}, \mathcal{A}_{\varphi_{k+1}} \varphi_{k+1} \rangle\rangle N^{-1}$.

It is well-known that Newton methods have a local nature. Hence, the convergence to a minimal solution can only be expected in a small neighbourhood of this solution, where the Hessian is positive definite. To circumvent this difficulty, inspired by the second-order derivative of the regularised Lagrangian \mathcal{L}_ω given in (4.15), the Riemannian Hessian can be parametrised by $\omega \in [0, 1]$ yielding the operator

$$\mathcal{H}_{\varphi,\omega} z = \mathcal{P}_{\varphi,L}(\mathcal{A}_\varphi z + \mathcal{B}_\varphi(z, \varphi) - \omega z \langle\langle \varphi, \mathcal{A}_\varphi \varphi \rangle\rangle N^{-1}), \quad z \in T_{\varphi_k} \mathcal{OB}_N(p, H).$$

For $\omega = 0$, this operator is positive definite on $T_{\varphi_k} \mathcal{OB}_N(p, H)$ due to Assumptions **A1** and **A2**, while for $\omega = 1$, we recover the Riemannian Hessian $\text{Hess}_L \mathcal{E}(\varphi)$. Therefore, we can view ω as a regularisation parameter. Solving the equation

$$\mathcal{H}_{\varphi_k, \omega_k} z_k = -\mathcal{R}_{\varphi_k} \varphi_k$$

instead of the Newton equation (5.7) leads to the *regularised Riemannian Newton* (regRN) method. In practice, we found that even for ω very close to 1, the convergence radius of the regRN method is much larger than that of the RN iteration. Comparing the regRN method with the LgrRGD iteration (5.5), in the case of weak inter-component interactions, the operator $\mathcal{G}_{\varphi,\omega}$ can be considered as an approximation to $\mathcal{H}_{\varphi,\omega}$, and, hence, (5.5) can be interpreted as a Riemannian quasi-Newton method. It should also be noted that our regRN method differs from the adaptive regularised Newton method presented in [57, 60], which approximates the Hessian by a quadratic functional.

In all above methods, scalar parameters such as the step size τ_k or the regularisation parameter ω_k can be chosen for each component individually, resulting in vector-valued parameters. Also, other Riemannian optimisation methods such as the Riemannian conjugate gradient, trust region, or quasi-Newton methods, see, e.g. [2, Chap. 7 & 8], can be extended to multicomponent infinite-dimensional BEC models in a similar way by introducing a vector transport between the different tangent spaces.

6. CONVERGENCE ANALYSIS OF ENERGY-ADAPTIVE RIEMANNIAN GRADIENT DESCENT

This section aims to demonstrate the reliability that arises from the problem-adaptive choice of the metric in RGD schemes. For the eaRGD method, we adapt the global qualitative and local

quantitative convergence results of the single-component case [38, 41, 42] to the multicomponent model under Assumptions **A1** and **A2**. This reliability makes the method a prime choice for the globalisation of the other schemes, in particular, the potentially locally faster RN methods.

6.1. Global convergence. First, we collect some technical results that are needed to prove the global convergence of the eaRGD method (5.3).

Lemma 6.1. For all $\varphi \in \mathcal{OB}_N(p, H)$, $\mathbf{z} \in T_\varphi \mathcal{OB}_N(p, H)$, and $\tau \geq 0$, the Riemannian gradient $\text{grad}_a \mathcal{E}(\varphi)$ can be bounded by $\|\text{grad}_a \mathcal{E}(\varphi)\|_{a_\varphi} \leq \|\varphi\|_{a_\varphi}$ and the normalisation operator (5.1) satisfies

$$(6.1) \quad \|\mathcal{N}(\varphi + \tau \mathbf{z}) - (\varphi + \tau \mathbf{z})\|_{a_\varphi} \leq \frac{\tau^2}{2} \|N^{-1}\|_2 \|\mathbf{z}\|_L^2 \|\varphi + \tau \mathbf{z}\|_{a_\varphi}.$$

Proof. The estimate for the Riemannian gradient $\text{grad}_a \mathcal{E}(\varphi)$ follows from (4.13) by using the same arguments as in the proof of [28, Lem. 4.2]. The bound (6.1) can be proved analogously to [8, Prop. 3.11] and [28, Lem. 4.3]. \square

Lemma 6.2. Let Assumptions **A1** and **A2** be fulfilled. For all $\varphi, \mathbf{v} \in H$, it holds that

$$|\mathcal{E}(\varphi + \mathbf{v}) - \mathcal{E}(\varphi)| \leq \|\varphi\|_{a_\varphi} \|\mathbf{v}\|_{a_\varphi} + \frac{1}{2} \|\mathbf{v}\|_{a_\varphi}^2 + C_K \left(\|\varphi\|_H^2 \|\mathbf{v}\|_H^2 + \|\varphi\|_H \|\mathbf{v}\|_H^3 + \frac{1}{4} \|\mathbf{v}\|_H^4 \right)$$

with $C_K = C_4^4 \|K\|_2$ and C_4 as in (2.5).

Proof. We have

$$\begin{aligned} \mathcal{E}(\varphi + \mathbf{v}) - \mathcal{E}(\varphi) &= a_\varphi(\varphi, \mathbf{v}) + \frac{1}{2} a_\varphi(\mathbf{v}, \mathbf{v}) \\ &\quad + \int_\Omega (\varphi \circ \mathbf{v}) K(\varphi \circ \mathbf{v})^T + (\varphi \circ \mathbf{v}) K(\mathbf{v} \circ \mathbf{v})^T + \frac{1}{4} (\mathbf{v} \circ \mathbf{v}) K(\mathbf{v} \circ \mathbf{v})^T \, dx. \end{aligned}$$

Therefore,

$$\begin{aligned} |\mathcal{E}(\varphi + \mathbf{v}) - \mathcal{E}(\varphi)| &\leq \|\varphi\|_{a_\varphi} \|\mathbf{v}\|_{a_\varphi} + \frac{1}{2} \|\mathbf{v}\|_{a_\varphi}^2 + \|K\|_2 \|\varphi\|_{[L^4(\Omega)]^p}^2 \|\mathbf{v}\|_{[L^4(\Omega)]^p}^2 \\ &\quad + \|K\|_2 \|\varphi\|_{[L^4(\Omega)]^p} \|\mathbf{v}\|_{[L^4(\Omega)]^p}^3 + \frac{1}{4} \|K\|_2 \|\mathbf{v}\|_{[L^4(\Omega)]^p}^4. \end{aligned}$$

Using the Sobolev embedding inequality (2.5), we then obtain the required estimate. \square

Lemma 6.3. Let Assumptions **A1** and **A2** be fulfilled. For $\varphi \in H$, let \mathcal{A}_φ be the operator defined in (2.9) with the corresponding bilinear form a_φ being coercive. Then for any $\mathbf{v} \in H$ with $\mathbf{v} \geq 0$, the p -frame $\mathcal{A}_\varphi^{-1} \mathbf{v}$ only has non-negative components, i.e., $\mathcal{A}_\varphi^{-1} \mathbf{v} \geq 0$.

Proof. First, we observe that $\mathcal{A}_\varphi^{-1} \mathbf{v}$ is the unique minimiser of the convex cost functional

$$\mathcal{F}(\mathbf{u}) = \frac{1}{2} a_\varphi(\mathbf{u}, \mathbf{u}) - (\mathbf{v}, \mathbf{u})_L, \quad \mathbf{u} \in H.$$

Further, due to $\mathbf{v} \geq 0$ and $(\mathbf{v}, \mathbf{u})_L \leq (\mathbf{v}, |\mathbf{u}|)_L$ for all $\mathbf{u} \in H$, we obtain that $\mathcal{F}(|\mathcal{A}_\varphi^{-1} \mathbf{v}|) \leq \mathcal{F}(\mathcal{A}_\varphi^{-1} \mathbf{v})$. This immediately implies that $\mathcal{A}_\varphi^{-1} \mathbf{v} = |\mathcal{A}_\varphi^{-1} \mathbf{v}| \geq 0$. \square

The following theorem shows that the iterates of the eaRGD method (5.3) are uniformly bounded and the energy functional \mathcal{E} decays for sufficiently small step sizes.

Theorem 6.4 (Energy decay). *Let $\{\varphi_k\}_{k=0}^\infty \subset \mathcal{OB}_N(p, H)$ be a sequence generated by the eaRGD method (5.3). Then there exist constants $C_0 > 0$ and $0 < C_\tau \leq 1$ depending on Ω , d , $\|K\|_2$, and $\|\varphi_0\|_{a_{\varphi_0}}$ such that for any step size $0 < \tau_{\min} \leq \tau_k \leq \tau_{\max} \leq C_\tau$ and any $k \geq 0$, the following relations hold:*

- (i) $\|\varphi_k\|_{a_{\varphi_k}} \leq C_0$,
- (ii) $\mathcal{E}(\varphi_k) - \mathcal{E}(\varphi_{k+1}) \geq \frac{1}{2} \tau_{\min} \|\text{grad}_a \mathcal{E}(\varphi_k)\|_{a_{\varphi_k}}^2$.

Proof. We prove the estimates by mathematical induction adapting the proof of [28, Th. 3.1] to the multicomponent setting and the energy-adaptive norm.

Set $C_0 = (2 + C_K \|\varphi_0\|_H^2)^{1/2} \|\varphi_0\|_{a_{\varphi_0}}$ with C_K as defined in Lemma 6.2. For $k = 0$, we obviously have $\|\varphi_0\|_{a_{\varphi_0}} \leq C_0$. Now assume that (i) holds for $0, 1, \dots, k$. Define $\mathbf{g}_k = \text{grad}_a \mathcal{E}(\varphi_k)$, $\tilde{\varphi}_k = \varphi_k - \tau_k \mathbf{g}_k$, and

$$\mathbf{r}_k = \varphi_{k+1} - \tilde{\varphi}_k = \mathcal{N}(\varphi_k - \tau_k \mathbf{g}_k) - (\varphi_k - \tau_k \mathbf{g}_k).$$

Then using Lemma 6.1 and (2.4), we estimate $\|\mathbf{g}_k\|_{a_{\varphi_k}} \leq C_0$, $\|\tilde{\varphi}_k\|_{a_{\varphi_k}} \leq 2C_0$, and

$$\|\mathbf{r}_k\|_{a_{\varphi_k}} \leq \frac{\tau_k^2}{2} \|N^{-1}\|_2 \|\mathbf{g}_k\|_L^2 \|\tilde{\varphi}_k\|_{a_{\varphi_k}} \leq \tau_k^2 C_N \|\mathbf{g}_k\|_{a_{\varphi_k}}^2$$

with $C_N = C_0 C_2^2 \|N^{-1}\|_2$. It further follows from Lemma 6.2 and its proof with appropriately chosen φ and \mathbf{v} that

$$\begin{aligned} |\mathcal{E}(\varphi_k - \tau_k \mathbf{g}_k) - \mathcal{E}(\varphi_k) - a_{\varphi_k}(\varphi_k, -\tau_k \mathbf{g}_k)| &\leq \tau_k^2 \left(\frac{1}{2} + \frac{9}{4} C_K C_0^2\right) \|\mathbf{g}_k\|_{a_{\varphi_k}}^2, \\ |\mathcal{E}(\tilde{\varphi}_k) - \mathcal{E}(\tilde{\varphi}_k + \mathbf{r}_k)| &\leq \tau_k^2 C_1 \|\mathbf{g}_k\|_{a_{\varphi_k}}^2 \end{aligned}$$

with $C_1 = 2C_0 C_N + \frac{1}{2} C_0^2 C_N^2 + C_K(4C_0^4 C_N^2 + 2C_0^5 C_N^3 + \frac{1}{4} C_0^6 C_N^4)$. Using these estimates and the relation $a_{\varphi_k}(\varphi_k, \mathbf{g}_k) = \|\mathbf{g}_k\|_{a_{\varphi_k}}^2$, we have

$$\begin{aligned} \mathcal{E}(\varphi_k) - \mathcal{E}(\varphi_{k+1}) &\geq \tau_k a_{\varphi_k}(\varphi_k, \mathbf{g}_k) - |\mathcal{E}(\tilde{\varphi}_k) - \mathcal{E}(\tilde{\varphi}_k + \mathbf{r}_k)| \\ &\quad - |\mathcal{E}(\varphi_k - \tau_k \mathbf{g}_k) - \mathcal{E}(\varphi_k) - a_{\varphi_k}(\varphi_k, -\tau_k \mathbf{g}_k)| \\ &\geq \tau_k \|\mathbf{g}_k\|_{a_{\varphi_k}}^2 - \tau_k^2 \left(\frac{1}{2} + \frac{9}{4} C_K C_0^2 + C_1\right) \|\mathbf{g}_k\|_{a_{\varphi_k}}^2 \geq \frac{\tau_{\min}}{2} \|\mathbf{g}_k\|_{a_{\varphi_k}}^2, \end{aligned}$$

provided that $\tau_{\max}(\frac{1}{2} + \frac{9}{4} C_K C_0^2 + C_1) \leq \frac{1}{2}$, which is guaranteed by $\tau_{\max} \leq C_\tau$ for some sufficiently small C_τ . This proves (ii) and, in particular, $\mathcal{E}(\varphi_{k+1}) \leq \mathcal{E}(\varphi_k)$. In order to show (i) for $k+1$, we estimate

$$\begin{aligned} \|\varphi_{k+1}\|_{a_{\varphi_{k+1}}}^2 &= 2\mathcal{E}(\varphi_{k+1}) + \frac{1}{2} \int_{\Omega} (\varphi_{k+1} \circ \varphi_{k+1}) K(\varphi_{k+1} \circ \varphi_{k+1})^T dx \leq 4\mathcal{E}(\varphi_{k+1}) \\ &\leq 4\mathcal{E}(\varphi_0) \leq 2\|\varphi_0\|_H^2 + \|K\|_2 \|\varphi_0\|_{[L^4(\Omega)]^p}^4 \leq (2 + C_K \|\varphi_0\|_H^2) \|\varphi_0\|_{a_{\varphi_0}}^2. \quad \square \end{aligned}$$

In order to guarantee the feasibility of the eaRGD iteration (5.3) in the case when K has negative entries, we need to ensure that \mathcal{A}_{φ_k} is invertible in every iteration. This can be achieved by shifting $\hat{a}_{\varphi_k}(\mathbf{v}, \mathbf{w}) = a_{\varphi_k}(\mathbf{v}, \mathbf{w}) + C(\mathbf{v}, \mathbf{w})_L$ with a sufficiently large constant $C > 0$ which can be chosen due to Theorem 6.4 independently of φ_k . In fact, in the three-dimensional case, taking $C \geq \hat{C}_0^8 C_4^8 C_6^6 \|K\|_2^4$ with $\hat{C}_0 = \|\varphi_0\|_H$ for $k = 0$ and $\hat{C}_0 = (2 + C_K \|\varphi_0\|_H^2)^{1/2} \|\varphi_0\|_{a_{\varphi_0}}$ otherwise, we obtain similarly to Theorem 6.4 that $\|\varphi_k\|_{\hat{a}_{\varphi_0}} \leq \hat{C}_0$ for all $k \geq 0$. Then, by Proposition 2.2, the bilinear form \hat{a}_{φ_k} is coercive for all $k \geq 0$ and, hence, the corresponding operator is invertible. The cases $d = 1, 2$ can be treated analogously.

We are now ready to prove the global convergence result for the eaRGD iteration.

Theorem 6.5 (Global convergence to the ground state). *Let Assumptions A1 and A2 be fulfilled. Let $\{\varphi_k\}_{k=0}^\infty \subset \mathcal{OB}_N(p, H)$ be a sequence generated by the eaRGD method (5.3) with step sizes $0 < \tau_{\min} \leq \tau_k \leq \tau_{\max} \leq C_\tau \leq 1$ as in Theorem 6.4, and a starting guess $\varphi_0 \in \mathcal{OB}_N(p, H)$ with $\varphi_0 \geq 0$. Then this sequence converges strongly in H to the unique ground state $\varphi_* \geq 0$.*

Proof. Starting with $\varphi_0 \geq 0$, we apply Lemma 6.3 recursively. Given $\varphi_k \geq 0$, we get

$$\begin{aligned} \tilde{\varphi}_k &= \varphi_k - \tau_k (\varphi_k - \mathcal{A}_{\varphi_k}^{-1} \varphi_k N \langle \varphi_k, \mathcal{A}_{\varphi_k}^{-1} \varphi_k \rangle^{-1}) \\ &= (1 - \tau_k) \varphi_k + \tau_k \mathcal{A}_{\varphi_k}^{-1} \varphi_k N \langle \varphi_k, \mathcal{A}_{\varphi_k}^{-1} \varphi_k \rangle^{-1} \geq 0. \end{aligned}$$

This then implies $\varphi_{k+1} = \tilde{\varphi}_k \langle \tilde{\varphi}_k, \tilde{\varphi}_k \rangle^{-1/2} N^{1/2} \geq 0$. Hence, the eaRGD iteration (5.3) preserves the non-negativity of the components.

By using Proposition 3.2 and the uniform boundedness of $\{\varphi_k\}$ shown in Theorem 6.4, similarly to [41, Th. 4.9 & Th. 5.1], we can prove that there exists a subsequence $\{\varphi_{k_l}\}$ converging strongly in L and H to a ground state $\varphi_* \in \mathcal{OB}_N(p, H)$ with $\varphi_* \geq 0$ and $\mathcal{E}(\varphi_*) = \lim_{k \rightarrow \infty} \mathcal{E}(\varphi_k)$. Let Λ_* denote

the associated Lagrange multiplier. Then for any $\varphi \in \mathcal{OB}_N(p, H)$, we have

$$a_{\varphi_*}(\varphi_*, \varphi_*) = (\varphi_* \Lambda_*, \varphi_*)_L = \sum_{j=1}^p N_j \lambda_{*,j} = \sum_{j=1}^p \|\varphi_j\|_{L^2(\Omega)}^2 \lambda_{*,j} = (\varphi \Lambda_*, \varphi)_L.$$

Hence, due to the definition of the smallest eigenvalues of the operators $\mathcal{A}_{\varphi_*,j}$ for $j = 1, \dots, p$, and the matrix K , it holds that

$$\begin{aligned} \mathcal{E}(\varphi) - \mathcal{E}(\varphi_*) &= \frac{1}{2}(a_{\varphi_*}(\varphi, \varphi) - a_{\varphi_*}(\varphi_*, \varphi_*)) \\ &\quad + \frac{1}{4} \int_{\Omega} (\varphi \circ \varphi) K (\varphi \circ \varphi)^T - 2(\varphi_* \circ \varphi_*) K (\varphi \circ \varphi)^T + (\varphi_* \circ \varphi_*) K (\varphi_* \circ \varphi_*)^T dx \\ &= \frac{1}{2} a_{\varphi_*}(\varphi - \varphi_*, \varphi - \varphi_*) - \frac{1}{2} ((\varphi - \varphi_*) \Lambda_*, \varphi - \varphi_*)_L \\ &\quad + \frac{1}{4} \int_{\Omega} (\varphi \circ \varphi - \varphi_* \circ \varphi_*) K (\varphi \circ \varphi - \varphi_* \circ \varphi_*)^T dx \\ &\geq \frac{\lambda_{\min}(K)}{4} \int_{\Omega} (\varphi \circ \varphi - \varphi_* \circ \varphi_*) (\varphi \circ \varphi - \varphi_* \circ \varphi_*)^T dx \\ &= \frac{\lambda_{\min}(K)}{4} \sum_{j=1}^p \int_{\Omega} (|\varphi_j|^2 - |\varphi_{*,j}|^2)^2 dx. \end{aligned}$$

The above relation with $\varphi = \varphi_k = (\varphi_{k,1}, \dots, \varphi_{k,p})$ implies that

$$\sum_{j=1}^p \int_{\Omega} (|\varphi_{k,j}|^2 - |\varphi_{*,j}|^2)^2 dx \leq \frac{4}{\lambda_{\min}(K)} (\mathcal{E}(\varphi_k) - \mathcal{E}(\varphi_*)) \xrightarrow{k \rightarrow \infty} 0.$$

Finally, taking into account that $\varphi_k \geq 0$ and $\varphi_* \geq 0$, we conclude that the whole sequence $\{\varphi_k\}$ converges strongly to φ_* in L as well as in H . \square

6.2. Local convergence. Our goal is to characterise the local convergence rate of the eaRGD iteration (5.3) with constant step size $\tau_k = \tau$ and element-wise non-negative interaction matrix K . To this end, we observe that this iteration can equivalently be written as the fixed point iteration $\varphi_{k+1} = \psi_{\tau}(\varphi_k)$ with the mapping $\psi_{\tau}: H \rightarrow H$,

$$\psi_{\tau}(\varphi) = \tilde{\psi}_{\tau}(\varphi) \langle \tilde{\psi}_{\tau}(\varphi), \tilde{\psi}_{\tau}(\varphi) \rangle^{-1/2} N^{1/2},$$

where $\tilde{\psi}_{\tau}(\varphi) = (1 - \tau)\varphi + \tau \mathcal{A}_{\varphi}^{-1} \varphi N \langle \varphi, \mathcal{A}_{\varphi}^{-1} \varphi \rangle^{-1}$. For a ground state $\varphi_* \in \mathcal{OB}_N(p, H)$, we have $\tilde{\psi}_{\tau}(\varphi_*) = \varphi_* = \psi_{\tau}(\varphi_*)$ showing that φ_* is a fixed point of ψ_{τ} . Proving that the spectral radius of the Fréchet derivative $D\psi_{\tau}(\varphi_*)$, denoted by $\varrho_* := \varrho(D\psi_{\tau}(\varphi_*))$, is smaller than 1, local convergence with rate ϱ_* follows from Ostrowski's theorem, see, e.g., [5, Prop. 1].

To proceed, we introduce the mappings $\zeta(\varphi) = \mathcal{A}_{\varphi}^{-1} \varphi$ and $\Xi(\varphi) = \langle \varphi, \zeta(\varphi) \rangle^{-1}$. Their directional derivatives at any $\varphi \in H \setminus \{\mathbf{0}\}$ along $\mathbf{v} \in H$ are given by

$$\begin{aligned} D\zeta(\varphi)[\mathbf{v}] &= \mathcal{A}_{\varphi}^{-1} \mathbf{v} - \mathcal{A}_{\varphi}^{-1} \mathcal{B}_{\varphi}(\mathbf{v}, \mathcal{A}_{\varphi}^{-1} \varphi), \\ D\Xi(\varphi)[\mathbf{v}] &= -(\langle \mathbf{v}, \mathcal{A}_{\varphi}^{-1} \varphi \rangle + \langle \varphi, \mathcal{A}_{\varphi}^{-1} \mathbf{v} - \mathcal{A}_{\varphi}^{-1} \mathcal{B}_{\varphi}(\mathbf{v}, \mathcal{A}_{\varphi}^{-1} \varphi) \rangle) \langle \varphi, \mathcal{A}_{\varphi}^{-1} \varphi \rangle^{-2}. \end{aligned}$$

Since the linear operators $D\zeta(\varphi)$ and $D\Xi(\varphi)$ are both continuous in a neighbourhood of φ_* , which excludes the zero element, $\zeta(\varphi)$ and $\Xi(\varphi)$ are Fréchet differentiable in this neighbourhood. This implies that $\tilde{\psi}_{\tau}(\varphi) = (1 - \tau)\varphi + \tau \zeta(\varphi) N \Xi(\varphi)$ and $\psi_{\tau}(\varphi)$ are also Fréchet differentiable in a neighbourhood of φ_* . In particular, evaluating $\zeta(\varphi)$, $\Xi(\varphi)$ and their derivatives at the ground state φ_* and taking into account that $\mathcal{A}_{\varphi_*}^{-1} \varphi_* = \varphi_* \Lambda_*^{-1}$ with $\Lambda_* = \langle \varphi_*, \mathcal{A}_{\varphi_*}^{-1} \varphi_* \rangle N^{-1}$, we obtain that

$$\begin{aligned} \zeta(\varphi_*) &= \varphi_* \Lambda_*^{-1}, & D\zeta(\varphi_*)[\mathbf{v}] &= \mathcal{A}_{\varphi_*}^{-1} \mathbf{v} - \mathcal{A}_{\varphi_*}^{-1} \mathcal{B}_{\varphi_*}(\mathbf{v}, \varphi_* \Lambda_*^{-1}), \\ \Xi(\varphi_*) &= \Lambda_* N^{-1}, & D\Xi(\varphi_*)[\mathbf{v}] &= -(\langle \mathbf{v}, \varphi_* \rangle \Lambda_*^{-1} + \langle \varphi_*, \mathcal{A}_{\varphi_*}^{-1} \mathbf{v} - \mathcal{A}_{\varphi_*}^{-1} \mathcal{B}_{\varphi_*}(\mathbf{v}, \varphi_* \Lambda_*^{-1}) \rangle) \Lambda_*^2 N^{-2}. \end{aligned}$$

Then the derivatives of $\tilde{\psi}_\tau$ and ψ_τ at φ_* are computed as

$$\begin{aligned} D\tilde{\psi}_\tau(\varphi_*)[\mathbf{v}] &= (1 - \tau)\mathbf{v} + \tau \left(D\zeta(\varphi_*)[\mathbf{v}]N\Xi(\varphi_*) + \zeta(\varphi_*)ND\Xi(\varphi_*)[\mathbf{v}] \right), \\ D\psi_\tau(\varphi_*)[\mathbf{v}] &= D\tilde{\psi}_\tau(\varphi_*)[\mathbf{v}] \langle \tilde{\psi}_\tau(\varphi_*), \tilde{\psi}_\tau(\varphi_*) \rangle^{-1/2} N^{1/2} \\ &\quad - \tilde{\psi}_\tau(\varphi_*) \langle \tilde{\psi}_\tau(\varphi_*), \tilde{\psi}_\tau(\varphi_*) \rangle^{-3/2} \langle D\tilde{\psi}_\tau(\varphi_*)[\mathbf{v}], \tilde{\psi}_\tau(\varphi_*) \rangle N^{1/2} \\ &= D\tilde{\psi}_\tau(\varphi_*)[\mathbf{v}] - \varphi_* \langle D\tilde{\psi}_\tau(\varphi_*)[\mathbf{v}], \varphi_* \rangle N^{-1}. \end{aligned}$$

We now consider the following linear eigenvalue problem: find an eigenfunction $\mathbf{v}_{\tau,i} \in H$ and an eigenvalue $\mu_{\tau,i} \in \mathbb{R}$ such that

$$(6.2) \quad D\psi_\tau(\varphi_*)[\mathbf{v}_{\tau,i}] = \mu_{\tau,i}\mathbf{v}_{\tau,i}.$$

We show that all eigenfunctions of $D\psi_\tau(\varphi_*)$ corresponding to nonzero eigenvalues belong to the tangent space $T_{\varphi_*}\mathcal{OB}_N(p, H)$.

Lemma 6.6. Let Assumptions **A1** and **A2** be fulfilled and let $\varphi_* \in \mathcal{OB}_N(p, H)$ be a ground state. Then all eigenfunctions $\mathbf{v}_{\tau,i}$ of (6.2) corresponding to $\mu_{\tau,i} \neq 0$ satisfy $\mathbf{v}_{\tau,i} \in T_{\varphi_*}\mathcal{OB}_N(p, H)$.

Proof. For all $\mathbf{v} \in H$, we have

$$\begin{aligned} \langle D\psi_\tau(\varphi_*)[\mathbf{v}], \varphi_* \rangle &= \langle D\tilde{\psi}_\tau(\varphi_*)[\mathbf{v}], \varphi_* \rangle - \langle \varphi_* \langle D\tilde{\psi}_\tau(\varphi_*)[\mathbf{v}], \varphi_* \rangle N^{-1}, \varphi_* \rangle \\ &= \langle D\tilde{\psi}_\tau(\varphi_*)[\mathbf{v}], \varphi_* \rangle - \langle \varphi_*, \varphi_* \rangle \langle D\tilde{\psi}_\tau(\varphi_*)[\mathbf{v}], \varphi_* \rangle N^{-1} = 0_p. \end{aligned}$$

From (6.2), we hence obtain for all eigenfunctions $\mathbf{v}_{\tau,i} \in H$ of $D\psi_\tau(\varphi_*)$ that

$$0_p = \langle D\psi_\tau(\varphi_*)[\mathbf{v}_{\tau,i}], \varphi_* \rangle = \mu_{\tau,i} \langle \mathbf{v}_{\tau,i}, \varphi_* \rangle.$$

This yields $\langle \mathbf{v}_{\tau,i}, \varphi_* \rangle = 0$ or, equivalently, $\mathbf{v}_{\tau,i} \in T_{\varphi_*}\mathcal{OB}_N(p, H)$ whenever $\mu_{\tau,i} \neq 0$. \square

Since zero eigenvalues are not relevant for the spectral radius of $D\psi_\tau(\varphi_*)$, we restrict the eigenvalue problem (6.2) to $T_{\varphi_*}\mathcal{OB}_N(p, H)$. In order to estimate ϱ_* , we first investigate an auxiliary linear eigenvalue problem: find $\mathbf{v}_i \in T_{\varphi_*}\mathcal{OB}_N(p, H)$ with $\langle \mathbf{v}_i, \mathbf{v}_i \rangle = I_p$ and $\mu_i \in \mathbb{R}$ such that

$$(6.3) \quad \mathcal{A}_{\varphi_*}^{-1}(\mathbf{v}_i - \mathcal{B}_{\varphi_*}(\mathbf{v}_i, \varphi_*\Lambda_*^{-1}))\Lambda_* = \mu_i\mathbf{v}_i.$$

The following lemma provides estimates for the eigenvalues μ_i .

Lemma 6.7. Let Assumptions **A1** and **A2** be fulfilled and let $\varphi_* \in \mathcal{OB}_N(p, H)$ be a ground state. Then all eigenvalues μ_i of (6.3) are real and satisfy

$$\mu_i \leq \frac{\sum_{j=1}^p \lambda_1(\mathcal{A}_{\varphi_*,j})}{\sum_{j=1}^p \lambda_2(\mathcal{A}_{\varphi_*,j})} < 1.$$

If, additionally, all entries of the interaction matrix K are non-negative, then $\mu_i > -2$ for all $i \in \mathbb{N}$.

Proof. It immediately follows from (6.3) that

$$\mu_i \langle \mathcal{A}_{\varphi_*}\mathbf{v}_i, \mathbf{v}_i \rangle = (\mathbf{v}_i\Lambda_*, \mathbf{v}_i)_L - \langle \mathcal{B}_{\varphi_*}(\mathbf{v}_i, \varphi_*\Lambda_*^{-1})\Lambda_*, \mathbf{v}_i \rangle = (\mathbf{v}_i\Lambda_*, \mathbf{v}_i)_L - \langle \mathcal{B}_{\varphi_*}(\mathbf{v}_i, \varphi_*), \mathbf{v}_i \rangle$$

and, hence, the μ_i are real. Furthermore, the Courant–Fischer theorem implies together with the orthogonality $\langle \mathbf{v}_i, \varphi_* \rangle = 0$ that

$$\langle \mathcal{A}_{\varphi_*}\mathbf{v}_i, \mathbf{v}_i \rangle = \sum_{j=1}^p \langle \mathcal{A}_{\varphi_*,j}v_{i,j}, v_{i,j} \rangle \geq \sum_{j=1}^p \lambda_2(\mathcal{A}_{\varphi_*,j}) \|v_{i,j}\|_{L^2(\Omega)}^2 = \sum_{j=1}^p \lambda_2(\mathcal{A}_{\varphi_*,j}),$$

where $v_{i,j}$ denotes the j -th component of \mathbf{v}_i . Then Proposition 3.2 together with $\langle \mathcal{B}_{\varphi_*}(\mathbf{v}_i, \varphi_*), \mathbf{v}_i \rangle \geq 0$ yields that

$$\mu_i = \frac{(\mathbf{v}_i\Lambda_*, \mathbf{v}_i)_L - \langle \mathcal{B}_{\varphi_*}(\mathbf{v}_i, \varphi_*), \mathbf{v}_i \rangle}{\langle \mathcal{A}_{\varphi_*}\mathbf{v}_i, \mathbf{v}_i \rangle} \leq \frac{(\mathbf{v}_i, \mathbf{v}_i\Lambda_*)_L}{\langle \mathcal{A}_{\varphi_*}\mathbf{v}_i, \mathbf{v}_i \rangle} \leq \frac{\sum_{j=1}^p \lambda_1(\mathcal{A}_{\varphi_*,j})}{\sum_{j=1}^p \lambda_2(\mathcal{A}_{\varphi_*,j})} < 1$$

due to $\lambda_1(\mathcal{A}_{\varphi_*,j}) < \lambda_2(\mathcal{A}_{\varphi_*,j})$ for $j = 1, \dots, p$. On the other hand, we can estimate

$$-\mu_i \leq \frac{\langle \mathcal{B}_{\varphi_*}(\mathbf{v}_i, \varphi_*), \mathbf{v}_i \rangle}{\langle \mathcal{A}_{\varphi_*}\mathbf{v}_i, \mathbf{v}_i \rangle} = \frac{2 \int_{\Omega} (\varphi_* \circ \mathbf{v}_i) K(\varphi_* \circ \mathbf{v}_i)^T dx}{\|\mathbf{v}_i\|_H^2 + \int_{\Omega} (\varphi_* \circ \varphi_*) K(\mathbf{v}_i \circ \mathbf{v}_i)^T dx} < 2.$$

The last inequality follows from

$$\int_{\Omega} (\varphi_* \circ \mathbf{v}_i) K(\varphi_* \circ \mathbf{v}_i)^T dx \leq \int_{\Omega} (\varphi_* \circ \varphi_*) K(\mathbf{v}_i \circ \mathbf{v}_i)^T dx,$$

provided that all entries of the interaction matrix K are non-negative. \square

We are now ready to prove that the eaRGD method (5.3) converges locally linear in H to the ground state φ_* and to specify the convergence rate.

Theorem 6.8 (Local convergence rate). *Let Assumptions A1 and A2 be fulfilled and let K be component-wise non-negative. Further, let $\varphi_* \in \mathcal{OB}_N(p, H)$ be a ground state and the eigenvalues μ_i of (6.3) be ordered decreasingly in magnitude, i.e., $|\mu_1| \geq |\mu_2| \geq \dots$. Then the spectral radius $\varrho_* = \varrho(D\psi_\tau(\varphi_*))$ satisfies*

$$(6.4) \quad \varrho_* < 1 \quad \text{for all } \tau \in \begin{cases} (0, \tau_*), & \text{if } \mu_1 > 0, \\ (0, \frac{2}{1+|\mu_1|}), & \text{if } \mu_1 < 0, \end{cases}$$

where

$$\tau_* = \frac{2 \sum_{j=1}^p \lambda_2(\mathcal{A}_{\varphi_*, j})}{\sum_{j=1}^p (\lambda_1(\mathcal{A}_{\varphi_*, j}) + \lambda_2(\mathcal{A}_{\varphi_*, j}))} > 1.$$

Furthermore, for every $\epsilon > 0$, there exists a neighbourhood \mathcal{U}_ϵ of φ_* in $\mathcal{OB}_N(p, H)$ and a positive constant C_ϵ such that for all starting functions $\varphi_0 \in \mathcal{U}_\epsilon$, the sequence $\{\varphi_k\}$ generated by the eaRGD method (5.3) with the constant step size $\tau_k = \tau$ fulfills

$$\|\varphi_k - \varphi_*\|_H \leq C_\epsilon |\varrho_* + \epsilon|^k \|\varphi_0 - \varphi_*\|_H \quad \text{for all } k \geq 1,$$

meaning that the eaRGD iteration (5.3) converges locally linear with rate ϱ_* .

Proof. Let $\mu_{\tau, i} \neq 0$ be an eigenvalue of $D\psi_\tau(\varphi_*)$ and $\mathbf{v}_{\tau, i} \in T_{\varphi_*} \mathcal{OB}_N(p, H)$ be the corresponding eigenfunction. Then for all $\mathbf{w} \in T_{\varphi_*} \mathcal{OB}_N(p, H)$, (6.2) and the formulae of the directional derivatives imply

$$\begin{aligned} \mu_{\tau, i} (\mathbf{v}_{\tau, i}, \mathbf{w})_L &= (D\psi_\tau(\varphi_*)[\mathbf{v}_{\tau, i}], \mathbf{w})_L = (D\tilde{\psi}_\tau(\varphi_*)[\mathbf{v}_{\tau, i}], \mathbf{w})_L \\ &= (1 - \tau)(\mathbf{v}_{\tau, i}, \mathbf{w})_L + \tau (\mathcal{A}_{\varphi_*}^{-1}(\mathbf{v}_{\tau, i} - \mathcal{B}_{\varphi_*}(\mathbf{v}_{\tau, i}, \varphi_* \Lambda_*^{-1})) \Lambda_*, \mathbf{w})_L. \end{aligned}$$

This shows that $\mu_{\tau, i} \neq 0$ is an eigenvalue of $D\psi_\tau(\varphi_*)$ if and only if $\mu_i = (\mu_{\tau, i} - 1 + \tau)/\tau$ is an eigenvalue of (6.3). Lemma 6.7 yields that $-2 < \mu_1 < 1$. Then using the same arguments as in the proof of [42, Lem. 5.8], we obtain that the spectral radius of $D\psi_\tau(\varphi_*)$ defined as $\varrho_* = \max_{i \in \mathbb{N}} |1 - \tau + \tau \mu_i|$ satisfies (6.4). Therefore, the local convergence estimate follows from Ostrowski's theorem [5, Prop. 1]. \square

Remark 6.9. Since $\tau_* > 1$ and $1 + |\mu_1| < 3$, the restriction for τ in (6.4) can be replaced by a stronger condition $\tau \in (0, \frac{2}{3}]$, which is much simpler to verify than (6.4).

Despite the favorable global convergence and local linear convergence rate for the eaRGD method presented above, the convergence analysis of other Riemannian optimisation methods for multicomponent BECs remains largely unexplored, particularly concerning local quantitative convergence results. Previously, the preconditioned L^2 -RGD method has been studied in [54] for Hartree–Fock and Kohn–Sham problems. More recently, RGD methods with a canonical H^1 -metric have been rigorously analyzed in [28]. Additionally, RN methods have been numerically proven to exhibit local quadratic convergence for Gross–Pitaevskii and Kohn–Sham problems [9]; see also [62] for the convergence analysis of the RN scheme for the discretised simplified Kohn–Sham model. However, the generalisation of these convergence results to multicomponent BECs is non-trivial and far beyond the scope of this paper.

7. FINITE ELEMENT DISCRETISATION

Due to the general infinite-dimensional formulation of our optimisation schemes, we may employ any appropriate spatial discretisation technique to discretise the minimisation problem (2.3) and the associated NLEVP (3.2). This includes (mixed) finite elements, multiscale, spectral, or pseudospectral methods [15, 23, 34, 40]. For illustration purposes, a finite element discretisation with $n \in \mathbb{N}$ degrees of freedom is considered in the following, which is also used in numerical experiments

in Section 8. Let $\Phi = [\phi_1, \dots, \phi_p]$, $U = [u_1, \dots, u_p]$, and $W = [w_1, \dots, w_p]$ denote the discrete tuples with $\phi_j, u_j, w_j \in \mathbb{R}^n$, $j = 1, \dots, p$, corresponding to the components of the p -frames φ , \mathbf{u} and \mathbf{w} , respectively. Note that, here and in the following, ϕ_j , u_j and w_j will always refer to the discrete vectors in \mathbb{R}^n rather than their continuous counterparts in $H_0^1(\Omega)$ considered in the previous sections.

The discretised version of the minimisation problem (2.3) takes the form

$$\min_{\Phi \in \mathcal{OB}_{N,M}(p,n)} E(\Phi),$$

where the generalised oblique matrix manifold is given by

$$\mathcal{OB}_{N,M}(p,n) = \{\Phi \in \mathbb{R}^{n \times p} : \text{ddiag}(\Phi^T M \Phi) = N\}$$

and the discretised energy functional reads

$$E(\Phi) = \sum_{j=1}^p \phi_j^T \left(\frac{1}{2} S + \frac{1}{2} M_{V_j} + \frac{1}{4} M_{\rho_j(\Phi)} \right) \phi_j.$$

Here, M is the L^2 -mass matrix, S is the stiffness matrix, $M_{\rho_j(\Phi)} = \sum_{i=1}^p \kappa_{ij} M_{\phi_i \phi_i}$ with the discretised density functions $\rho_j(\Phi)$, and M_{V_j} and $M_{\phi_i \phi_i}$ are weighted mass matrices, where $\phi_i \phi_i$ should be understood as the element-wise product.

The discrete version of the bilinear form a_φ in (2.7) reads

$$a_\Phi(U, W) = \langle A_\Phi(U), W \rangle_M = \text{trace}(W^T M A_\Phi(U))$$

with the linear operator $A_\Phi: \mathbb{R}^{n \times p} \rightarrow \mathbb{R}^{n \times p}$ given by

$$A_\Phi(U) = [M^{-1} A_{\Phi,1} u_1, \dots, M^{-1} A_{\Phi,p} u_p],$$

where $A_{\Phi,j} = S + M_{V_j} + M_{\rho_j(\Phi)}$ for $j = 1, \dots, p$. Furthermore, the discretisation of the operator $\mathcal{B}_\varphi(\mathbf{u}, \varphi)$ in (3.5) is given by

$$B_\Phi(U, \Phi) = \left[M^{-1} \sum_{j=1}^p B_{\Phi,1j} u_j, \dots, M^{-1} \sum_{j=1}^p B_{\Phi,pj} u_j \right]$$

with $B_{\Phi,ij} = 2\kappa_{ij} M_{\phi_i \phi_j}$ for $i, j = 1, \dots, p$. We equip the tangent space

$$T_\Phi \mathcal{OB}_{N,M}(p,n) = \{Z \in \mathbb{R}^{n \times p} : \text{ddiag}(\Phi^T M Z) = 0_p\}$$

with a Riemannian metric which follows the product structure

$$g_\Phi^\times(Z, Y) = \text{trace}(Z^T M G_\Phi^\times(Y)), \quad Z, Y \in T_\Phi \mathcal{OB}_{N,M}(p,n),$$

where the operator $G_\Phi^\times(Y) = [M^{-1} G_{\Phi,1} y_1, \dots, M^{-1} G_{\Phi,p} y_p]$ acts column-wise and the matrices $G_{\Phi,j} \in \mathbb{R}^{n \times n}$ are symmetric positive definite. As discussed in Section 4, this restriction to metrics, that act on all components independently, allows expressions that are both simple and computationally efficient. The g_Φ^\times -orthogonal projection onto the tangent space $T_\Phi \mathcal{OB}_{N,M}(p,n)$ is given by

$$\begin{aligned} P_\Phi^\times(U) &= U - (G_\Phi^\times)^{-1}(\Phi) \text{ddiag}(\Phi^T M U) (\text{ddiag}(\Phi^T M (G_\Phi^\times)^{-1}(\Phi)))^{-1} \\ &= \left[u_1 - \frac{\phi_1^T M u_1}{\phi_1^T M G_{\Phi,1}^{-1} M \phi_1} G_{\Phi,1}^{-1} M \phi_1, \dots, u_p - \frac{\phi_p^T M u_p}{\phi_p^T M G_{\Phi,p}^{-1} M \phi_p} G_{\Phi,p}^{-1} M \phi_p \right]. \end{aligned}$$

Further, the discretisation of $\mathcal{R}_\varphi \mathbf{u}$ is given by

$$R_\Phi(U) = \left[M^{-1} R_{\Phi,1} u_1, \dots, M^{-1} R_{\Phi,p} u_p \right]$$

with $R_{\Phi,j} = A_{\Phi,j} - \sigma_j M$ and $\sigma_j = \frac{\phi_j^T A_{\Phi,j} \phi_j}{N_j}$ for $j = 1, \dots, p$. Using the above definitions, the corresponding Riemannian gradient of E then takes the form

$$\text{grad} E(\Phi) = P_\Phi^\times((G_\Phi^\times)^{-1}(R_\Phi(\Phi))) = [G_{\Phi,1}^{-1}(R_{\Phi,1} - \theta_1 M) \phi_1, \dots, G_{\Phi,p}^{-1}(R_{\Phi,p} - \theta_p M) \phi_p],$$

where

$$\theta_j = \frac{\phi_j^T M G_{\Phi,j}^{-1} R_{\Phi,j} \phi_j}{\phi_j^T M G_{\Phi,j}^{-1} M \phi_j}, \quad j = 1, \dots, p.$$

Using $G_{\Phi,j} = M$, $G_{\Phi,j} = A_{\phi,j}$ or $G_{\Phi,j} = G_{\Phi,\omega,j} = A_{\phi,j} + B_{\Phi,jj} - \omega\sigma_j M$, we obtain the Riemannian gradients with respect to the discrete L^2 -, energy-adaptive or Lagrangian-based metric, respectively. The discretisation of the Riemannian Hessian with respect to the L^2 -metric is given by

$$\text{Hess}_M E(\Phi)[Z] = M^{-1} \left[P_{\Phi,M,1} \left(R_{\Phi,1} z_1 + \sum_{j=1}^p B_{\Phi,1j} z_j \right), \dots, P_{\Phi,M,p} \left(R_{\Phi,p} z_p + \sum_{j=1}^p B_{\Phi,pj} z_j \right) \right]$$

with the projectors $P_{\Phi,M,j} = I - \frac{1}{N_j} M \phi_j \phi_j^T$. These expressions can be used to construct the discrete counterparts of the Riemannian optimisation schemes presented in Section 5.

It should be noted that the global convergence results for the eaRGD method no longer hold in the finite-dimensional case because our particular choice of the finite element discretisation does not satisfy a discrete maximum principle. Achieving this would require a slightly modified, stabilised scheme as proposed in [37]. However, in practice, unless specifically triggered, a violation of the maximum principle and potential convergence to an excited state from a positive initial guess will typically not be observed. We also refer to [27], for recent convergence results of the RGD method based on the H^1 -metric for a discretised single-component BEC.

8. NUMERICAL EXPERIMENTS

We report on numerical experiments for two test examples in 1D and 2D domains, aiming at comparing the performance of the different Riemannian optimisation schemes presented in Section 5. For the spatial discretisation, we use the finite element method with bi-quadratic elements on a quadrilateral mesh of width h . We impose Neumann boundary conditions instead of the Dirichlet boundary conditions discussed above, but due to the strong trapping potentials in the models, all values on the boundary are sufficiently close to zero in all experiments. The implementation was done in the Julia programming language using the package `Ferrite.jl` for the finite element discretisation. The source code is available in the GitHub repository <https://github.com/MaHermann/Riemannian-coupledGPE> and relies on the following parameter and design choices:

- **Stopping criterion:** We terminate the iterations once the norm of the residual $\text{res}_k = (\text{trace}(R_{\Phi_k}(\Phi_k)^T M R_{\Phi_k}(\Phi_k)))^{1/2}$ falls below the tolerance $\text{tol} = 10^{-8}$.
- **Initial guess:** For all schemes, we use a consistent initial guess Φ_0 computed by the alternating eaRGD method, where each component is initialised by 1. Iterations continue until the residual norm, as defined by the stopping criterion, falls below 10^{-2} in the 1D case and 10^{-4} in the 2D case.
- **Step size:** To maintain transparency in the comparison between methods, we use a constant step size of $\tau_k = 1$ for all RGD methods presented here. This approach allows a clear evaluation of the inherent convergence properties of each method, without introducing variability due to the interplay between method choice and adaptive step size strategies. In particular, all methods show stable convergence without the need for smaller step sizes, except for the LgrRGD scheme applied to the 2D problem with random potential (see below). The use of an adaptive step size strategy, such as a non-monotone line search combined with the alternating Barzilai–Borwein step size strategy [59, 61], could further improve the optimisation performance, but we leave this method-specific refinement for future work.
- **Linear system solvers:** For solving linear systems in Riemannian gradient and Newton direction calculations, we employ the preconditioned conjugate gradient method with the preconditioner determined from the ILU decomposition of $A_{0,j} = S + M_{V_j}$ and an adaptive residual tolerance tol_{CG} for the 1D system and 10tol_{CG} for the 2D system, where the latter has a weaker nonlinearity, allowing for less accurate solutions. Here, $\text{tol}_{CG} = \text{res}_k$ as defined above for the Newton-type methods, and the residual norm for the individual components for the RGD methods. For the computation of the initial guess Φ_0 by using the alternating eaRGD method, we take a tolerance of $1.5 \cdot 10^{-8} \text{tol}_{CG}$ in the linear systems.
- **Regularisation parameters:** In the LgrRGD method, we take $\omega_k = 1$, as discussed in Section 5.1.3. In the regRN method, we use $\omega_k = 0.99$, which proves to be enough to provide convergence in the cases where the RN method (which corresponds to $\omega_k = 1$) does not converge.

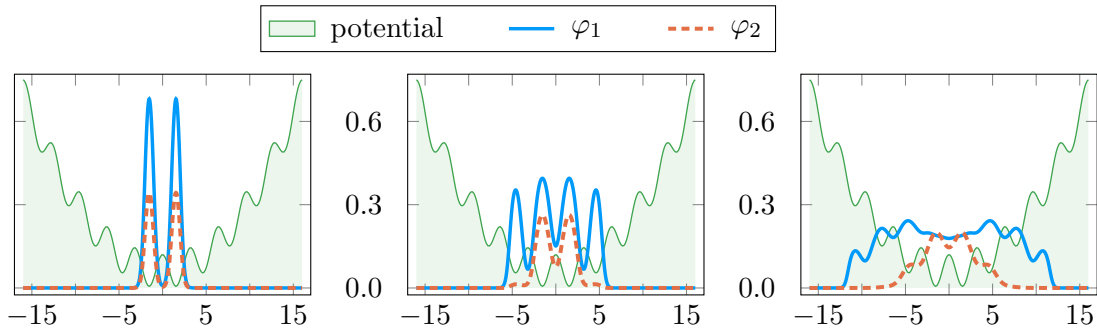


FIGURE 8.1. Two-component BEC: potential and components of the ground state for $\beta = 10, 100, 1000$ (from left to right). The potential is rescaled by a factor of 0.0025 for plotting purposes.

Although the most canonical performance measure is probably the number of outer iterations to a given stopping criterion, in practice other measures may play a more important role. For example, a Newton step takes on average much longer than a gradient step, so it makes sense to also compare the total CPU time required. Since the computational time depends to a large extent on the implementation and the hardware used, we also report the average number of matrix–vector multiplications with $n \times n$ matrices per optimisation step, which, together with the assembly of the finite element matrices discussed below, are the most expensive operations in all optimisation schemes. Together, these performance measures provide sufficient insight into the individual strengths of the different optimisation methods.

Each optimisation step requires the assembly of the finite element matrices $M_{\phi_i \phi_j}$. In the eaRGD and LgrRGD methods, only the p matrices $M_{\phi_i \phi_i}$ are needed, while the RN and regRN methods require all $p(p+1)/2$ combinations to compute the (regularised) Riemannian Hessian. In the cases below with $p = 2, 3$, this amounts to a factor of at most two, but it should be taken into account when applying the optimisation schemes to models with a large number of components.

Note that in both examples below, the interaction matrix K has non-negative entries, so by Remark 2.3 there is no need to shift A_{Φ} to ensure its invertibility.

8.1. Two-component BEC in 1D. First, we consider a well-known benchmark example from the literature, see, e.g., [14, 43]. It describes a two-component BEC on $\Omega = [-16, 16]$ with the potentials

$$V_1(x) = V_2(x) = 2 \left(\frac{1}{2} x^2 + 24 \cos^2(x) \right)$$

and the interaction parameters $\kappa_{11} = 2.08\beta$, $\kappa_{22} = 1.94\beta$ and $\kappa_{12} = \kappa_{21} = 2\beta$, where different values for $\beta > 0$ can be chosen. By renormalisation, we can assume, without loss of generality, that $N_1 + N_2 = 1$, so we take $N_1 = \alpha$ and $N_2 = 1 - \alpha$ with $\alpha \in (0, 1)$. The differences in parameters compared to the earlier works result from the choice of constants in the energy and the fact that the interaction matrix K used there is not positive definite and therefore does not fit in the setting of this paper, so we use a slightly larger κ_{11} . In the following, we fix $\alpha = 0.8$ and perform experiments for $\beta = 10, 100, 1000$ to examine how the strength of the nonlinearity affects the individual optimisation methods.

We choose a finite element mesh width of $h = 32 \cdot 2^{-10}$, resulting in $n = 2049$ degrees of freedom. The initialisation with the alternating eaRGD method takes 5, 9, and 17 iterations for $\beta = 10, 100$, and 1000, respectively. Figure 8.1 presents the potential and the resulting ground state components. The convergence history of the residual norms for different optimisation methods and different values of β is shown in Figure 8.2. To illustrate the advantage of the alternating variant of the LgrRGD scheme, in addition to the convergence history for the alternating versions, we also include the residual plots for the non-alternating schemes for the case $\beta = 100$. Further details on the number of outer iterations and the average number of matrix–vector multiplications in an optimisation step are given in Table 8.1. We do not provide time measurements for these one-dimensional experiments, as they are all in the order of seconds, where precompilation of the Julia code and other factors such as implementation details and processor load dominate.

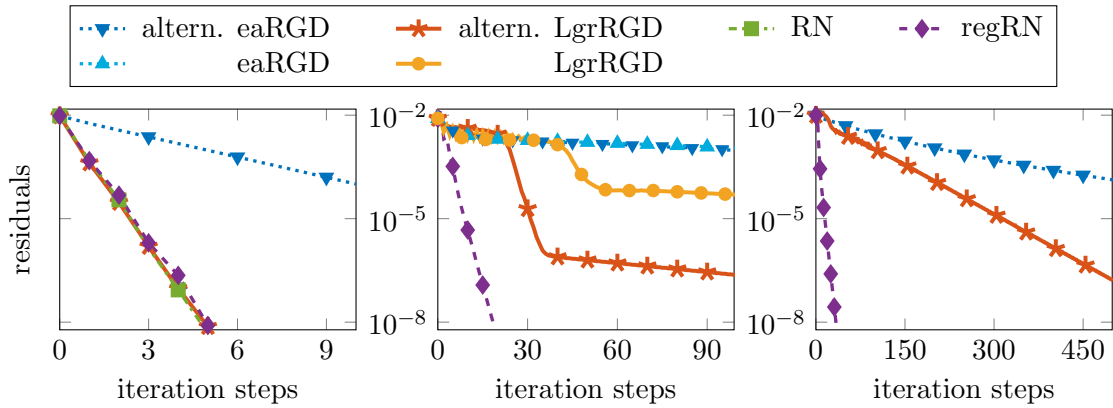


FIGURE 8.2. Two-component BEC: convergence history of the residuals for $\beta = 10, 100, 1000$ (from left to right). For $\beta = 100$, the non-alternating versions of the eaRGD and LgrRGD methods are shown as well.

TABLE 8.1. Two-component BEC: performance measures for different optimisation methods

| | outer iter. | aver. matr.-vec. mult. per iter. | outer iter. | matr.-vec. mult. per iter. | outer iter. | matr.-vec. mult. per iter. |
|----------------|--------------|----------------------------------|---------------|----------------------------|----------------|----------------------------|
| | $\beta = 10$ | | $\beta = 100$ | | $\beta = 1000$ | |
| altern. eaRGD | 31 | 12.1 | 1147 | 14.0 | 2225 | 20.3 |
| altern. LgrRGD | 5 | 30.4 | 259 | 60.0 | 629 | 106.6 |
| RN | 5 | 20.0 | - | - | - | - |
| regRN | 5 | 20.0 | 19 | 53.3 | 34 | 131.9 |

Figure 8.2 and Table 8.1 show that the regRN method converges in significantly fewer iterations than the alternating eaRGD method for all three parameter values of β and that the alternating LgrRGD method is competitive to both the RN and regRN methods for $\beta = 10$. For strong interactions ($\beta = 100, 1000$), the RN method does not converge to the ground state, as the initial value is too far away. This could be fixed by more initial iterations with the reliable eaRGD method or by regularisation with the regRN method.

8.2. Three-component BEC in 2D. As a second example, we consider a three-component BEC model on the unit square $\Omega = [0, 1]^2$, uniformly partitioned with mesh width $h = 2^{-10}$ in each direction, resulting in $n = 4\,198\,401$ degrees of freedom, a much larger problem size than in the previous 1D example. The interaction parameters are $\kappa_{11} = 0.5$, $\kappa_{22} = 5$, $\kappa_{33} = 10$ and $\kappa_{ij} = 1$ otherwise, while the number of particles is $N_1 = N_2 = N_3 = 1$.

We consider two cases: a periodic potential and a piecewise random potential, both taking values in $\{0, 2^{12}\}$ and varying on a length scale of $\epsilon = 2^{-6}$. In both cases, to enforce small values at the boundary, we additionally add a trapping potential

$$V_{\text{trap}}(x_1, x_2) = 10^6 \max\{(2x_1 - 1)^{40}, (2x_2 - 1)^{40}\}.$$

The initialisation takes 3 and 4 eaRGD steps for the periodic and random potentials, respectively.

In our experiments, we observed that for the periodic potential, all optimisation schemes converge to the same ground state. For the random potential, however, only the eaRGD method reliably provides the ground state, while the other schemes find excited states with higher energy, even with the relatively small initialisation residual of 10^{-4} .

Comparing the computed ground states for the two models shown in Figure 8.3, we see that for the periodic potential, the ground state remains spread over the entire domain, while for the random potential, the condensate undergoes localisation, see [4, 6, 7] for related results for single-component BECs. These works also justify that both cases are extremely computationally challenging, as the spectral gaps in the lower energy spectrum are very small and scale like ϵ , which explains the need for very accurate initial estimates to avoid approaching excited states of similar energy levels.

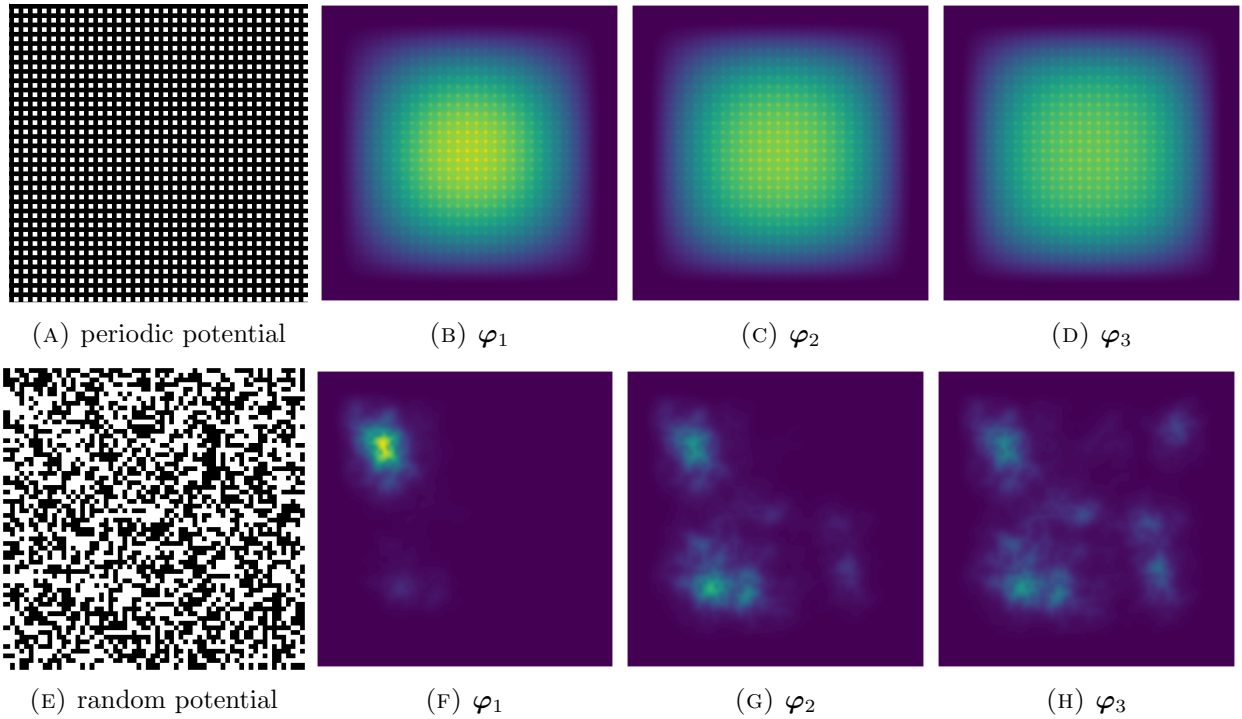


FIGURE 8.3. Three-component BEC: random and periodic potentials and components of the ground states computed with the alternating eaRGD method. For the potentials, we do not depict the additional trapping potential that is used to enforce the homogeneous Dirichlet boundary conditions.

TABLE 8.2. Three-component BEC: performance measures for different optimisation methods.

| | outer iter. | aver. matr.-vec. mult. per iter. | CPU time (minutes) | energy | residual |
|--------------------|-------------|----------------------------------|--------------------|--------|------------|
| periodic potential | | | | | |
| altern. eaRGD | 206 | 42.8 | 87 | 4582.2 | 9.9016e-09 |
| altern. LgrRGD | 4 | 665.2 | 24 | 4582.2 | 4.3065e-10 |
| RN | 4 | 1249.5 | 25 | 4582.2 | 6.3026e-11 |
| regRN | 5 | 954.6 | 25 | 4582.2 | 7.5963e-09 |
| random potential | | | | | |
| altern. eaRGD | 1503 | 63.5 | 773 | 2332.1 | 9.9942e-09 |

The performance measures including the computational time together with the final energy values and residual norms for the convergent methods are collected in Table 8.2. It can be seen that for the periodic potential, the alternating LgrRGD, RN, and regRN methods, which are based on the second-order information, significantly outperform the alternating eaRGD method both in terms of the number of outer iterations and the computational time. For the random potential, as reported above, only the alternating eaRGD method provides the ground state, but requires a prohibitively large number of iterations to achieve small target residuals and is computationally very expensive. Therefore, a combination of the eaRGD and RN methods, exploiting both the global convergence guarantees of the former and the fast local convergence speed of the latter, seems to be a promising approach to compute ground states in an efficient way. In addition, the development of better preconditioners to reduce the large number of inner iterations and suitable step size control strategies to speed up convergence could further improve the computational performance of the optimisation algorithms.

9. CONCLUSION

In this paper, we have introduced a general framework for computing the ground state of multi-component Bose–Einstein condensates using Riemannian optimisation methods on the infinite-dimensional generalised oblique manifold. This problem is formulated as an energy minimisation problem with mass conservation constraints for each condensate component. We have established existence and uniqueness results for the ground state on a bounded spatial domain and linked it to the coupled Gross–Pitaevskii eigenvalue problem. In addition, we have explored the Riemannian structure of the generalised oblique manifold by defining several Riemannian metrics and computing essential geometric tools such as gradients and Hessians.

By incorporating first- and second-order information of the energy functional, we have constructed appropriate metrics that allow preconditioning within Riemannian optimisation, which, combined with improvements through alternating iterations, significantly enhances optimisation performance. Our qualitative global and quantitative local convergence results for the energy-adaptive Riemannian gradient descent method provide a robust basis for further exploration of complex multicomponent Bose–Einstein condensation phenomena in quantum systems.

Acknowledgement. The authors would like to thank Jonas Püschel for fruitful and constructive discussions on important implementation aspects.

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(R. Altmann) INSTITUTE OF ANALYSIS AND NUMERICS, OTTO VON GUERICKE UNIVERSITY MAGDEBURG, UNIVERSITÄTSPLATZ 2, 39106 MAGDEBURG, GERMANY
Email address: robert.altmann@ovgu.de

(M. Hermann) INSTITUTE OF MATHEMATICS, UNIVERSITY OF AUGSBURG, UNIVERSITÄTSSTRASSE 12A, 86159 AUGSBURG, GERMANY
Email address: martin.hermann@uni-a.de

(D. Peterseim, T. Stykel) INSTITUTE OF MATHEMATICS & CENTRE FOR ADVANCED ANALYTICS AND PREDICTIVE SCIENCES (CAAPS), UNIVERSITY OF AUGSBURG, UNIVERSITÄTSSTRASSE 12A, 86159 AUGSBURG, GERMANY
Email address: daniel.peterseim@uni-a.de
Email address: tatjana.stykel@uni-a.de