



# Hybrid preconditioning for iterative diagonalization of ill-conditioned generalized eigenvalue problems in electronic structure calculations <sup>☆</sup>

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## ABSTRACT

The iterative diagonalization of a sequence of large ill-conditioned generalized eigenvalue problems is a computational bottleneck in quantum mechanical methods employing a nonorthogonal basis for *ab initio* electronic structure calculations. We propose a hybrid preconditioning scheme to effectively combine global and locally accelerated preconditioners for rapid iterative diagonalization of such eigenvalue problems. In partition-of-unity finite-element (PUFE) pseudopotential density-functional calculations, employing a nonorthogonal basis, we show that the hybrid preconditioned block steepest descent method is a cost-effective eigensolver, outperforming current state-of-the-art global preconditioning schemes, and comparably efficient for the ill-conditioned generalized eigenvalue problems produced by PUFE as the locally optimal block preconditioned conjugate-gradient method for the well-conditioned standard eigenvalue problems produced by planewave methods.

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## 1. Introduction

First principles (*ab initio*) quantum mechanical simulations based on density functional theory (DFT) [21,24] are a vital component of research in condensed matter physics and molecular quantum chemistry. Using DFT, the many-body Schrödinger equation for the ground state properties of an interacting system of electrons and nuclei is reduced to the self-consistent solution of an effective single-particle Schrödinger equation, known as the Kohn–Sham equation:

$$\mathcal{H}\psi_i(r) = \left[ -\frac{1}{2}\nabla^2 + V_{\text{eff}}(r, \rho(r)) \right] \psi_i(r) = \varepsilon_i \psi_i(r), \quad (1)$$

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where  $\varepsilon_i$  are particle energies (eigenvalues) and  $\psi_i$  are the associated wavefunctions (eigenfunctions). The Hamiltonian  $\mathcal{H}$  consists of kinetic energy operator  $-\frac{1}{2}\nabla^2$  and effective potential operator  $V_{\text{eff}}(r, \rho(r))$ . The effective potential  $V_{\text{eff}}$  depends on the electronic charge density

$$\rho(r) = \sum_i f_i |\psi_i(r)|^2, \quad (2)$$

where  $0 \leq f_i \leq 2$  is the electronic occupation of state  $i$  and the sum is over all occupied states. Since  $\psi_i$  depends on  $V_{\text{eff}}$  which depends on  $\rho(r)$  which depends again on  $\psi_i$ , the Kohn–Sham equation (1) is a nonlinear eigenvalue problem.

The importance of *ab initio* calculations stems from their underlying quantum-mechanical nature, yielding insights inaccessible to experiment and robust, predictive power unattainable by more approximate empirical approaches. However, because *ab initio* calculations are computationally intensive, a vast range of real materials problems remain inaccessible by such accurate, quantum mechanical means. To address this limitation, there has been substantial effort in recent years to develop *ab initio* methods that use efficient, local bases in order to both reduce degrees of freedom and facilitate large-scale parallel implementation: augmented planewave plus local orbital (APW+lo) [48,49], atomic-orbital (AO), e.g., [3,8], and real-space methods [6,54,40] such as finite-difference [11,12,10], wavelet [13,2,17], finite-element (FE) [55,35], partition-of-unity finite element (PUFE) [53,37,36], and discontinuous Galerkin (DG) [26] methods, among many others, see for example [29].

In the vast majority of *ab initio* methods, the dominant computational cost is the iterative diagonalization of the sequence of large linear eigenvalue problems produced by the discretization of Eq. (1) in the chosen basis [42,25,59,41,40,60,57,39]. The linear eigenvalue problems produced by highly efficient physics based APW+lo, AO, and PUFE bases, while smaller than those of other bases, present a particular challenge as they are generalized eigenvalue problems with ill-conditioned coefficient matrices, and are much more difficult to precondition than those produced by conventional planewave based methods, due to the lack of diagonal dominance and absence of an efficient representation for the inverse Laplacian.

Here, building on prior work [58,47,33,1,39,7], we propose a *hybrid preconditioning scheme* for rapid iterative diagonalization of the sequence of ill-conditioned generalized Hermitian eigenvalue problems produced by modern orbital based electronic structure methods, such as APW+lo, AO, and PUFE. The hybrid preconditioning scheme effectively combines a global shifted-inverse preconditioner as in [33,1,7] and locally accelerated shifted-inverse preconditioners as in [58,47,33,1,39] that target eigenpairs of interest individually. The global preconditioner serves as sole preconditioner in early self-consistent iterations and as convergence accelerator for local preconditioners in subsequent iterations. We have conducted extensive tests of the proposed hybrid preconditioning scheme with the block steepest descent method in PUFE pseudopotential density functional calculations on a variety of systems, including the difficult case of triclinic metallic CeAl. This system has deep atomic potentials and 15 electrons per unit cell in valence, thus requiring the computation of many, strongly localized eigenfunctions, which in turn requires the addition of correspondingly many orbital enrichments in the PUFE electronic structure method. Our results reveal that in terms of average numbers of inner and outer iterations, the hybrid preconditioner performs markedly better than global or local preconditioners alone, and the resulting solver performs as well on the ill-conditioned generalized eigenvalue problems produced by the PUFE *ab initio* method as does the locally optimal block preconditioned conjugate-gradient (LOBPCG) method on well-conditioned *standard* eigenvalue problems produced by the planewave method.

The remainder of the paper is organized as follows. In Section 2, we outline the self-consistent field (SCF) procedure and iterative diagonalization process in an algebraic setting, and discuss the ill-conditioned generalized eigenvalue problems produced by the PUFE electronic structure method. In Section 3, we describe the hybrid preconditioning scheme and its use in the block steepest descent method. Implementation details are presented in Section 4. Numerical results are presented in Section 5 and we close with final remarks in Section 6.

## 2. SCF, iterative diagonalization, and ill-conditioned GHEPs

Electronic structure methods such as APW+lo, AO, and PUFE methods incorporate information from local atomic solutions to construct efficient bases for molecular or condensed matter calculations. This information is typically incorporated in the form of localized, atomic-like basis functions (orbitals), which generally leads to a nonorthogonal basis. Discretization of the Kohn–Sham equation (1) in such a basis then leads to a nonlinear algebraic eigenvalue problem

$$H(V_{\text{eff}})\Psi = S\Psi E, \quad (3)$$

where  $H(V_{\text{eff}})$  is the discrete KS-Hamiltonian matrix and consists of a local part  $H^{(\text{loc})}(V_{\text{eff}})$  and, when pseudopotentials [29] are employed, nonlocal part  $H^{(\text{nl})}$ :

$$H(V_{\text{eff}}) = H^{(\text{loc})}(V_{\text{eff}}) + H^{(\text{nl})}.$$

$H^{(\text{loc})}(V_{\text{eff}})$  is a Hermitian matrix which depends on the effective potential  $V_{\text{eff}}$ , which in turn depends on the electronic density  $\rho(r)$  computed from the eigenvectors  $\Psi$ .  $H^{(\text{nl})}$  is a low-rank Hermitian matrix associated with the nonlocal part of the pseudopotential.  $S$  is the overlap (Gram) matrix of the basis and is Hermitian positive-definite. The nonlocal matrix  $H^{(\text{nl})}$  and overlap matrix  $S$  are independent of  $V_{\text{eff}}$ , and hence do not depend on  $\rho(r)$  or  $\Psi$ . In condensed matter calculations, it is required to sample the Brillouin zone [29] at a sufficient number of  $\mathbf{k}$ -points, making the above matrices complex

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