

UCLA

UCLA Electronic Theses and Dissertations

Title

Development of a Superconducting Solver in Finite Differences

Permalink

<https://escholarship.org/uc/item/72w0k4n7>

ISBN

9798190929362

Author

Dhiraj, Maanasi Harini

Publication Date

2026-09-11

Peer reviewed|Thesis/dissertation

UNIVERSITY OF CALIFORNIA

Los Angeles

Development of a Superconducting
Solver in Finite Differences

A thesis submitted in partial satisfaction
of the requirements for the degree
Master of Science in Materials Science and Engineering

by

Maanasi H. Dhiraj

2026

ABSTRACT OF THE THESIS

Development of a Superconducting Solver in Finite Differences

by

Maanasi H. Dhiraj

Master of Science in Materials Science and Engineering

University of California, Los Angeles, 2026

Professor Amartya S. Banerjee, Chair

Superconductivity is a powerful phase in which materials conduct electricity with little to no resistance. Most studied superconducting materials show transition from the normal state under cryogenic temperatures. Computational approaches to studying superconducting candidate materials bridge theory and experiment, especially in the search for high temperature superconductors for applications in energy and transportation. Implementation of the superconducting functions in finite differences is the first step in efficient computational study of known and candidate materials with Superconducting Density Functional Theory. A one-dimensional prototype of a solver of the Bogoliubov de Gennes equations in real-space is presented for implementation with current density functional theory packages, such as the Matlab-Simulation Package for Ab-initio Real-space Calculations. The implemented numerical methods accelerate convergence of superconducting properties to a self-consistency residual tolerance of 10^{-9} . Verification of the model is shown through comparison with analytically expected results for a conventionally superconducting system and qualitative interpretation of the predicted density of states.

The thesis of Maanasi H. Dhiraj is approved.

Daniel Schwalbe-Koda

Md. Shafayat Hossain

Amartya S. Banerjee, Committee Chair

University of California, Los Angeles

2026

TABLE OF CONTENTS

Introduction	1
Background	2
Superconductivity	2
Microscopic Theory of Superconductivity	3
Superconducting Density Functional Theory	5
Method Development	7
Computational Implementation	7
Construction of the Bogoliubov de Gennes Hamiltonian	9
Post-Diagonalization Calculations for Continuum Solution	10
Numerical Methods for Self-Consistent Field	11
Results	13
Numerical Evaluation	15
Alignment with BCS Theory	18
Future Directions	20
Conclusion	20
References	22

LIST OF FIGURES

1	Comparison of Convergence of Linear and Pulay Mixing	15
2	Mesh-Convergence Study of Computed Gap Function with Different Finite Difference Orders. Δ_{ref} is calculated from a fine mesh of 0.02 with a finite difference template of order 12.	16
3	Validation of Numerically Computed Energy Dispersion with Discretized BCS Theory Analytical Solution for $\Delta = \frac{1}{3}\mu$	17
4	Magnitude of Mean-Field Gap vs Temperature Ratio to Superconducting Critical Temperature	18
5	Comparison of Density of States for Normal and Superconducting Systems . . .	19

ACKNOWLEDGMENTS

I am grateful to my advisor, Professor Amartya S. Banerjee for his supervision in pursuing the research topic and for crucial support in the debugging of the program used for this thesis. Through his guidance, I was able to apply materials science coursework from my undergraduate studies, numerical methods, and programming toward a current knowledge gap with real-world applications. I extend my sincere appreciation to Professor Md. Shafayat Hossain and Professor Daniel Schwalbe-Koda for their service on my thesis committee. I greatly benefited from their courses in solid state physics and computational materials science, respectively, and their useful feedback for a more informed perspective towards my research project.

I am indebted to my parents for their support, both tangible and intangible, throughout my studies. Thank you to the Graduate Writing Center for their year-round workshops and writing retreats. Thank you to the Graduate Office for streamlining the filing process and hosting helpful workshops and office hours. Thank you also to my friends for their kind encouragement and enthusiasm.

Acknowledgment of AI Usage: AI tools were consulted for gathering sources in the literature (Perplexity) and debugging (Claude Sonnet 5, GPT 5.6) in the refinement of the Bogoliubov de Gennes solver. The author is responsible for the text and analysis, with guidance from the thesis committee.

Introduction

Global population increases and present-day technological advancements, such as electric vehicles and artificial intelligence, place greater demands on the world's electricity supply. For the next five years, a projected annual increase of 3.6% in electricity needs places pressures on the energy grid [1]. Increased use of renewable and traditional energy sources provide the balance, but material solutions offer a long term strategy to mitigate the inevitable demands of future technologies and a growing global economy. Superconductivity is a powerful condensed matter phenomenon that offers efficiency through superconducting currents operating with no heat loss. Superconducting materials undergo a phase transition to a superconducting state, in which the material conducts with little to no electrical resistance.

However, practical use of experimentally studied superconducting materials requires sufficient cooling. At the time of this writing, the highest widely accepted superconducting temperature is 250 K, for a sample of lanthanum decahydride pressurized at 170 GPa [2]. To identify a practical superconductor for global needs, computational studies can relate material physics to superconductivity.

Density functional theory (DFT) remains a powerful simulation tool that enables first principles studies of materials at the electron scale. However, the original mathematical framework is based on materials in a normal phase. The development of superconducting density functional theory (SCDFT) incorporates additional equations and offers targeted study of material properties that may lead to the realization of higher temperature superconductors. The SCDFT formalism is especially useful for the study of candidates for high T_c superconductors, which have inhomogeneity in the form of crystalline defects to induce charge carriers [3].

In addition, the quantity of candidate materials to simulate requires development of computationally efficient methods. At present, the database SuperCon catalogs more than 13,000 distinct compositions, while the search space of unknown superconductors is unquantified

[4].

A few recent implementations of superconductivity with DFT packages use an orbital basis. This thesis discusses the implementation of the microscopic theory of superconductivity for a one-dimensional solver. This is a working prototype that uses a prescribed normal-state Hamiltonian but does not constitute a full implementation of SCDFT. The solver is implemented in finite differences and intended to work with M-SPARC, a DFT package numerically implemented in finite differences for efficient real-space calculations, in future work [5] [6] [7].

Background

Superconductivity

Superconductivity is the behavior of near zero electrical resistance exhibited by materials that undergo a superconducting phase transition at a critical temperature, T_c , specific to the material. In theory, superconducting currents may continue indefinitely, with some experiments suggesting a characteristic decay time of up to 10^5 years [8]. Such properties could enable efficient high-current transmission lines with low heat loss. Superconductors also possess strong magnetic properties, useful for applications such as magnetic resonance imaging and high speed rails operating with magnetic levitation. Scientific experiments especially benefit from superconductors in super ferric magnets for particle accelerators [9].

The development of superconductivity study began with the study of electrical resistance in cooled metals, such as mercury and niobium. Interest in room temperature superconductors motivates study of alloys and more novel combinations. Circuit components also benefit from unique combinations of superconductors, such as Josephson junctions, which tunnel Cooper pairs through the interface of two superconducting materials and provide lossless inductance [10].

Initial theories of superconductors, such as the London equations, related electromagnetic properties fields of a superconductor to a phenomenological parameter Λ , capturing the effect of the number density, n_s of superconducting electrons along with the mass, m , and electron charge, e . The London equation for electric field replaced Ohm's law for superconductors:

$$\frac{\partial}{\partial t}(\Lambda \mathbf{J}) = \mathbf{E}; \Lambda = \frac{m}{n_s e^2}$$

The London model approached an explanation of the stability of the superconducting current. The electric field accelerates the superconducting electrons. With zero electric field, the superconducting current remains steady, with no energy loss. However, investigation of the electron interactions requires further quantum mechanical study [11].

The Ginzburg-Landau Theory provides a phenomenological description of superconductivity in which a complex pseudo wavefunction, ψ , describes the superconducting electrons and acts as an order parameter. From a series expansion of the free energy, expressed in terms of ψ and $\nabla\psi$, the theory yields the differential equation for ψ :

$$\frac{1}{2m^*} \left(\frac{\hbar}{i} \nabla - \frac{e^*}{c} A \right)^2 \psi + \beta |\psi|^2 \psi = -\alpha(T) \psi$$

where m^* is the effective mass, $\hbar$ is the reduced Planck's constant, e^* is the effective electron charge, A is the magnetic vector potential, and α and β are expansion coefficients. The formalism is similar to the Schrodinger equation of a free particle, but the quadratic term captures the effect of the density of superconducting electrons, $n_s = |\psi(x)|^2$. The Ginzburg-Landau Theory provided a physically intuitive relation between the superconductivity phase transition and the quantum-mechanical nature of its charge carriers. With the development of theories that related superconductivity phenomena to electrons, more targeted study of electron coupling remained critical to study of material systems.

Microscopic Theory of Superconductivity

The basis of superconductivity is the coordinated motion of electrons. Bardeen, Cooper, and Schrieffer provided the microscopic theory of superconductivity, or BCS Theory, in

which conventional superconductivity arises from the pairing of electrons that glide with little resistance [12]. Cooper proposed that these electron pairs are the charge carriers in the superconducting current [13]. The energy associated with this electron pairing is represented by an energy gap or gap function, Δ . In conventional superconductivity, the pairing of the electrons is explained by lattice vibrations creating positive ions that overcome electron-electron repulsion. This electron-phonon coupling gives rise to the Cooper pairs.

To relate superconductivity to the electron pairing, thermodynamic principles relate the free energy associated with the superconducting phase to the gap function. The Cooper pair formation produces instability in the Fermi sea of electrons. Multiple pairs condense into the ground state without restriction by the Pauli exclusion principle, since the bound pairs behave like bosons. The Cooper pairs condense until equilibrium is achieved. The gap function remains nonzero at this equilibrium state but becomes zero when the system is brought to the superconducting transition temperature, T_c .

Minimization of the Helmholtz energy associated with the phase transition yields the gap function in terms of the single-particle state, k :

$$\Delta_k = - \sum_{k'} V_{kk'} \frac{\Delta_{k'}}{2E_{k'}} \tanh\left(\frac{\beta E_{k'}}{2}\right)$$

Here, $V_{kk'}$ is the local attraction between the electron pair, and the energy states arise as $E_k = \sqrt{\epsilon_k^2 + |\Delta_k|^2}$ from the single-particle normal-state Hamiltonian's eigenenergies ϵ_k and the gap function Δ [14].

The BCS Theory not only offers a framework to explain pairing of electrons for superconductivity but also ties microscopic theory to the phenomenological Ginzburg-Landau Theory. A later derivation showed the Ginzburg-Landau Theory is a form of the BCS Theory at the critical temperature of phase transition, and that the order parameter, ψ , is proportional to the gap parameter, Δ .

Superconducting Density Functional Theory

Electron interactions establish material properties, and electronic structure calculations are especially effective for studying problems relating to ground and excited states [15]. Density Functional Theory (DFT) offers a computationally feasible framework for studying this many-body problem. Superconducting Density Functional Theory (SCDFT) incorporates the Bogoliubov de Gennes equations to solve the gap function computationally [3]. To incorporate superconductivity, the Bogoliubov de Gennes (BdG) equations provide a mathematical framework to relate paired electron states to the gap function [16] [17].

Bogoliubov de Gennes Equations

Normal density functional theory (DFT) captures standard electron behavior, but the Bogoliubov de Gennes (BdG) framework extends to superconducting systems by incorporating both the DFT Hamiltonian and the gap function, Δ [17]. To adapt BdG for DFT, we use the continuum model implemented in finite differences.

Initially, the tight-binding model suggest an intuitive discrete study of a material's lattice for real-space DFT [18]. However, to accurately represent the electronic structure in the BdG model and connect the BdG solver to the M-SPARC routine, we require the continuum model to resolve the electron-scale real-space implementation and appropriately match the eigenvalue energy scale.

For the single-electron Hamiltonian, the eigenvalue problem takes on a form such as

$$\xi_n w_n = \left(-\frac{\hbar^2}{2m}\nabla^2 + U_0(\mathbf{r}) - E_F\right)w_n$$

which captures the kinetic energy, external potential, and energy correction (with the Fermi level E_F as the reference).

For each energy solution ξ_n , there are at least 2 corresponding solutions $w_n = w_n(\mathbf{r})|\uparrow\rangle$ and $w_{\bar{n}} = w_n^*(\mathbf{r})|\downarrow\rangle$. An initial approach may propose a trial function that combines

the degenerate energy states, but the BdG derivation provides more freedom for this trial function. The BdG method allows solution of the electron-paired Hamiltonian in a magnetic field and yields lower energy solutions, also lowering the paired electrons' eigenstates w_n . Second quantization introduces the operators Ψ and Ψ^+ , which represent combinations of electron and hole creation and annihilation.

For the superconducting case, the effective Hamiltonian $\mathcal{H}_{\text{eff}}$ includes electron coupling under an external potential:

$$\mathcal{H}_{\text{eff}} = \int d\mathbf{r} \{ \Psi^\dagger(\mathbf{r}) \mathcal{H}_e \Psi(\mathbf{r}) + U(\mathbf{r}) \Psi^\dagger(\mathbf{r}) \Psi(\mathbf{r}) + \Delta(\mathbf{r}) \Psi^\dagger(\mathbf{r} \uparrow) \Psi^\dagger(\mathbf{r} \downarrow) + \Delta^*(\mathbf{r}) \Psi(\mathbf{r} \downarrow) \Psi(\mathbf{r} \uparrow) \}$$

with the corresponding general form single-particle Hamiltonian

$$\mathcal{H}_e = -\frac{[\frac{\hbar}{i}\nabla_{\mathbf{r}} + \frac{e}{c}\mathbf{A}(\mathbf{r})]^2}{2m_e} - e\phi(\mathbf{r}) + \alpha\mu_B H(\mathbf{r}) - E_F$$

Here, the Hamiltonian $\mathcal{H}_e$ captures the kinetic energy, external potential (in terms of both the vector $\mathbf{A}(\mathbf{r})$ and scalar $\phi(\mathbf{r})$ potentials, which can be varied for a gauge invariant solution), chemical potential μ , magnetic field $H(\mathbf{r})$, and energy correction [18]. The Nambu basis implementation achieves the pairing function by coupling the spin-up quasi-electron component $u(\mathbf{r})$ with the spin-down quasi-hole component $v(\mathbf{r})$. A series of transformations yield the BdG equations.

$$\begin{aligned} Eu(\mathbf{r}) &= [\mathcal{H}_e + U(\mathbf{r})]u(\mathbf{r}) + \Delta(\mathbf{r})v(\mathbf{r}) \\ Ev(\mathbf{r}) &= -[\mathcal{H}_e^* + U(\mathbf{r})]v(\mathbf{r}) + \Delta^*(\mathbf{r})u(\mathbf{r}) \end{aligned}$$

The resulting wavefunction components, $u(\mathbf{r})$ and $v(\mathbf{r})$, provide the electron- and hole-like amplitudes in the excitations of a superconductor. These amplitudes provide the self-consistent solution for the gap function.

Self-Consistent Field for Gap Function

To identify the correct gap function, use of a self-consistent approach allows iterative improvement on the initial guess. Solving the Hamiltonian in the BdG equations yields a

condition for a self-consistent gap function in one-dimension:

$$\Delta(\mathbf{r})_{\text{scf}} = +V \sum_n v_n^*(\mathbf{r}) u_n(\mathbf{r}) (1 - 2f_n)$$

with the Fermi-Dirac distribution $f_n = \frac{1}{\exp(\beta E_n) + 1}$ [17] Here, $v_n^* u_n$ is nonzero near the Fermi surface, so $\Delta(\mathbf{r})$ is a function of temperature. For study with the single-particle Hamiltonian, the Fermi-Dirac distribution represents the state occupation. Only in their bound state, the coupled electrons behave like bosons. The self-consistent gap function achieves minimization of a SCDF functional with respect to the anomalous density associated with superconductivity [3].

Achieving the correct form of the self-consistent gap function requires tuning of the effect of the local electron pairing potential. Using the continuum model, the local electron pairing potential is understood in terms of the pairing coefficient, g : $V(x, x') = -g\delta(x - x')$ [19]. Cooper pairs undergoing s-wave pairing, characteristic of conventional superconductors, have a net zero angular momentum, due to the symmetry of the orbitals involved [8]. Assuming a uniform, non-zero gap function arising from s-wave pairing, the pairing coefficient is expressed in terms of the normal eigenenergies and gap function:

$$\frac{1}{g} = \frac{1}{L} \sum_k \frac{1}{2E_k} \tanh\left(\frac{E_k}{2k_B T}\right)$$

After establishing the pairing coefficient, the self-consistent field approach uses this potential to determine the appropriate gap function.

Method Development

Computational Implementation

The quantum mechanical nature of solving the normal-state Hamiltonian alone requires time-consuming and memory-intensive computational runs. Numerical solution requires discretization of the governing equations and operators like the Hamiltonian. In the literature

of development of electronic structure solvers, there are three main approaches to discretization: plane waves, localized orbitals, and real-space implementations. Calculations using a plane wave basis represent the Hamiltonian as a dense matrix, due to the periodic potential arising from the lattice representation. The computational cost scales as $\mathcal{O}(n \log n)$, with use of a Fast Fourier Transform on each iteration [20].

Localized orbitals serve as an alternative basis, specific to atomic sites and requires storage of many indices for state labels, atomic orbitals, and localized functions. Sophisticated functions allow computational complexity to reduce to $\mathcal{O}(n)$ per iteration [21]. Determination of basis functions requires testing to optimize for a specific geometry, and convergence depends on different variables associated with a specific configuration [20].

Direct implementation of DFT in real-space uses finite differences to discretize the system. Real-space DFT provides natural execution on parallel computers due to the lack of localized functions [5]. Real-space methods produce larger but sparser matrices than the traditional plane wave-based DFT, allowing efficient calculations. Some calculations on sequential computers can run faster by an order of magnitude, compared to implementations with explicit bases [20].

A recent approach to SCDFT is a SIESTA-based solver that incorporated the BCS Theory through the BdG construction [22]. SIESTA is a DFT package implemented with an orbital basis, so the program requires storage of orbital and atomic site information to develop an orbital overlap matrix. The overlap matrix is incorporated in the BdG equations to form a generalized eigenvalue problem. This thesis discusses the construction of a BdG Hamiltonian solver for real-space implementation and study with a DFT package, such as M-SPARC [6] [7]. M-SPARC, the Matlab-Simulation Package for Ab-initio Real-space Calculations, provides efficient implementation of DFT methods in finite differences.

In addition, M-SPARC's program structure enables prototyping of variations on the foundational DFT method, which is especially beneficial to incremental development of SCDFT. To develop SCDFT, one must establish the original BdG Hamiltonian construction. Then,

numerical refinement of the self-consistent calculations will enable efficient convergence of the gap function. As higher dimensions are incorporated, the wavefunctions associated with the Cooper pairs have more degrees of freedom, leading to more complex behavior such as vortices of magnetic flux and mixed superconducting states, characteristic of Type II superconductors [8].

In the initial one-dimensional solver, a normal-state Hamiltonian incorporates kinetic energy and chemical potential in finite differences. The precision of the Laplacian operator, used for the second derivative in the normal-state Hamiltonian, is tuned with Fornberg coefficients [23]. Here, the one-dimensional BdG Hamiltonian allows study of superconducting in shapes such as nanowires, in which superconductivity corresponds to s-wave pairing. The implemented gap function assumes the local, isotropic pairing interaction and s-wave gap required for s-wave pairing.

Construction of the Bogoliubov de Gennes Hamiltonian

The Bogoliubov de Gennes (BdG) formulation of the Hamiltonian allows solution for the energy dispersion and corresponding eigenstates of a superconducting system.

$$\begin{pmatrix} H_0(k) - \mu & \Delta(k) \\ \Delta^*(-k) & (-H_0 + \mu)^* \end{pmatrix} \begin{pmatrix} u \\ v \end{pmatrix} = \varepsilon_i \begin{pmatrix} u \\ v \end{pmatrix}$$

Here, H_0 is the normal-state Hamiltonian, μ is the chemical potential, and Δ is the superconducting pairing potential. H_0 is initially discretized with a $N \times N$ matrix. It is assumed that the electronic states are sufficiently described by H_0 , and that effects such as inter-band hybridization may be ignored [24]. The corresponding BdG Hamiltonian is a $2N \times 2N$ block matrix. Assuming s-wave pairing, the block matrix is interpreted as the reduced form of a spin-singlet superconductor's Hamiltonian, in which spins are all paired and net spin is zero [25]. This is distinct from a spinless system.

At each iteration, the BdG solver establishes a single-particle Hamiltonian and a guess for the gap function. The SCDFE formalism requires minimization of a functional with respect to an anomalous density function. This is analogous to the minimization of the DFT energy functional with respect to the normal state electron density. In a fully self-consistent SCDFE implementation, the SCDFE functional is minimized with respect to both the normal and anomalous densities for a uniform treatment of the superconducting behavior [3]. In this thesis, a prototype of the superconducting self-consistent model, with a fixed normal-state Hamiltonian, is discussed as the foundation for a full SCDFE implementation in finite differences.

Post-Diagonalization Calculations for Continuum Solution

After the BdG matrix is diagonalized, the positive-energy states are filtered to avoid double-counting the eigenstates. Here, an absence of spin-orbit coupling and spin-flip scattering is assumed [18]. After choosing the positive window, a further cutoff window is established with the Fermi-Dirac distribution to determine which states contribute to the pairing.

The BdG matrix is diagonalized using MATLAB's `eig()` function, which produces vectors with Euclidean normalization. Converting u and v from the Euclidean-normalized eigenvectors to continuum amplitudes, introduces a factor of $\frac{1}{\sqrt{h}}$ for each wavefunction. To appropriately calculate the updated gap function, the coupling coefficient g is corrected with a factor of $\frac{1}{h}$:

$$\Delta(\mathbf{r})_{\text{scf}} = \frac{g}{h} \sum_n v_n^*(\mathbf{r}) u_n(\mathbf{r}) (1 - 2f_n)$$

Since the initial calibration of the coupling coefficient is mesh-independent, the correction factor corrects the effect of the mesh for a specific calculation. Once the self-consistent gap function is achieved, the local density of states is calculated by summation over the wavefunction amplitudes, adjusted with a chosen peak broadening parameter, η :

$$\rho(r, E) = \sum_n [|u_n(r)|^2 \eta(E - E_n) + |v_n(r)|^2 \eta(E + E_n)]$$

. Thus, implementation of the self-consistent field is important to probe further properties.

Numerical Methods for Self-Consistent Field

The gap function guess is incrementally improved by mixing the current iteration's gap function, Δ_i , with the gap function, Δ_{scf} , calculated from the current iteration's wavefunctions. Comparison of the self-consistent gap function with the current iteration yields the error, minimized in achievement of numerical convergence.

To achieve convergence of the self-consistent gap function, two different mixing schemes from the literature were implemented for comparison. Linear mixing, the most straightforward approach, allows an easy method for steady convergence: $\Delta_{m+1} = (1 - \alpha)\Delta_m + \alpha\Delta_{\text{scf}}$. Linear mixing averages the previous and newly calculated gap function values and converges slowly. The mixing parameter, α , damps the convergence and can require manual tuning.

The computational cost of the program is in the self-consistent field calculation, which involves diagonalizing the BdG matrix. It is important to reduce iterations required for convergence to the desired error tolerance. Pulay mixing, also known as Direct Inversion in the Iterative Subspace, rapidly increases the speed of convergence for self-consistent problems [26]. The efficiency of convergence arises from storage of the history of previous iterations' guesses and errors for the gap function values. Pulay mixing forms the optimal linear combination of previous iterations to minimize gap function error.

The development of self-consistent field iterations involves sophisticated combinations of different mixing schemes. Periodic Pulay mixing outperforms standard Pulay mixing for number of iterations required to converge [27]. Switching between linear and Pulay mixing reduces the residual at each step, avoiding a Pulay mixing history matrix of linearly dependent columns in B.

Algorithm Periodic Pulay Mixing for Gap Function Δ

Given the initial guess x_1 , function f_{scf} , s:= Pulay start, p:= Pulay frequency, α := Linear mixing factor

for all $k = 1, 2, \dots$ until convergence **do**

if $k \geq s$ AND $((k - s) \bmod p) == 0$ **then**

 Pulay Mixing

$$y_k = f_{\text{scf}}(x_k)$$

$$r_k = y_k - x_k$$

 Add x_k to gap history X, r_k to residual history R

$B_{ij} = \langle R_i, R_j \rangle$ for $i, j = 1, 2, \dots, n$ in $|R|$

$$\begin{bmatrix} B & -1 \\ -1^T & 0 \end{bmatrix} \begin{bmatrix} c \\ \lambda \end{bmatrix} = \begin{bmatrix} 0 \\ -1 \end{bmatrix}$$

 Solve for $c = (c_1, c_2, \dots, c_n)$ to form $x = \sum_i c_i X_i$

$$x_{k+1} = x_k + \beta x$$

else

 Linear Mixing

$$x_{k+1} = x_k + \alpha r_k$$

end if

end for

Length	40 Bohr
Number of Lattice Points	96
Finite Difference Order	4
Chemical Potential	1.0
Temperature (Low, Non-Zero Approximation)	0.02
Energy Cutoff	0.75
Cutoff Width (Smooth)	0.05
Pulay Start Iteration	5
Pulay Frequency	1
Gap Function Guess Δ_0	0.05
Calculated pairing coefficient g for Δ_0	1.9044
Linear Mixing Parameter α	0.35
Pulay Mixing Parameter β	0.85

Table: Default Solver Parameters

A table of default solver parameters used for the following results is provided. The solver is specifically designed for periodic boundary conditions. Deviations from the general parameters are explicitly stated, when applicable.

Results

The current BdG prototype works in atomic units, with quantities $\hbar = m = k_B = 1$. Physical parameters such as length and temperature were fixed across all runs. To achieve a superconducting gap, a chemical potential was applied to fill states beyond the band edge. To establish mesh-independent calculations, the coupling coefficient, g, was first calculated from the dispersion of the initial guess gap function, Δ_0 , in a mesh-independent calculation and held constant for subsequent gap function calculations of varied mesh size.

To verify the BdG solver's efficacy, convergence of the different mixing methods were first compared. Since this is a finite difference implementation, the convergence with different Laplacian stencils was also shown across coarse to fine mesh sizes.

To evaluate the BdG solver's implementation of BCS Theory, the calculated gap function's temperature dependence and energy dispersion were compared to expected results from the theory. In addition, the density of states shows the difference in band structure between the normal and superconducting states.

Numerical Evaluation

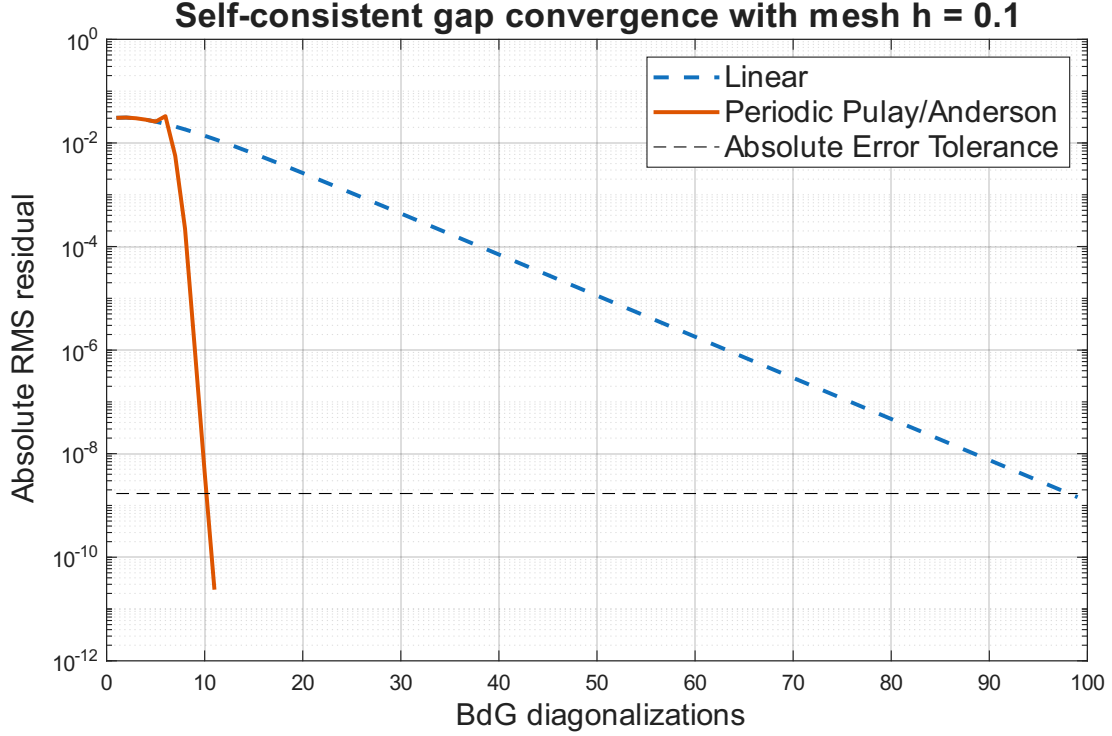


Figure 1: Comparison of Convergence of Linear and Pulay Mixing

Comparison of the linear mixing and periodic Pulay implementations for a fixed coarse mesh spacing of $h = 0.1$ shows the convergence of periodic Pulay within 11 iterations for an absolute self-consistent residual tolerance of 10^{-9} . To show comparison, the periodic Pulay mixer first performs 5 iterations of linear mixing and switches to Pulay mixing. Fig. 1 shows the linear mixing achieves the same convergence of the mixed solution in 91 iterations. For practical calculations, less frequent Pulay mixing is to ensure the residual history vectors do not become linearly dependent.

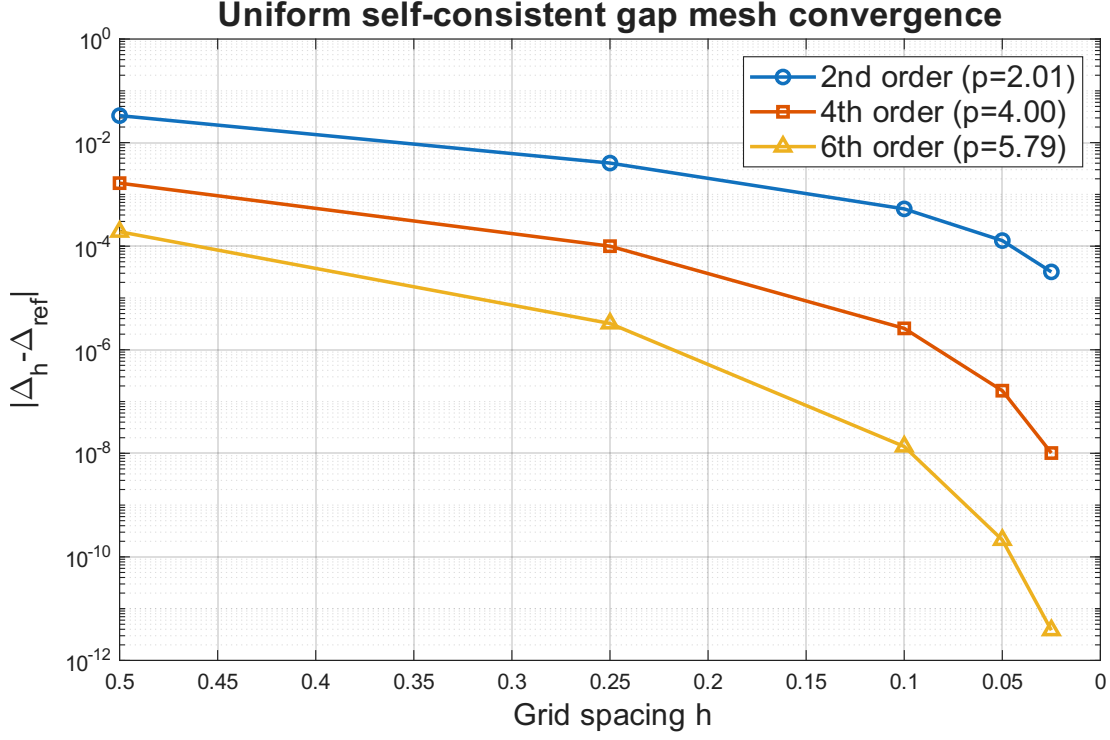


Figure 2: Mesh-Convergence Study of Computed Gap Function with Different Finite Difference Orders. Δ_{ref} is calculated from a fine mesh of 0.02 with a finite difference template of order 12.

To tune the precision of the BdG solver, both mesh and order of the finite difference were varied, and the calculated gap functions were compared to calculation with a fine mesh of $h = 0.02$ and finite difference stencil of order 12. The absolute error of each gap function from a calculation with coarser mesh is shown in Fig. 2. With increase in the order of the finite difference implementation, the absolute error of the gap function decreases by up to 1.5 orders of magnitude. The difference in convergence with mesh size increases with the choice of Laplacian stencil. For the one-dimensional model, a stencil of order n calculation requires $2n + 1$ relevant neighboring mesh points used for computing the central difference. Ultimately, use of a higher order finite difference stencil for a desired error tolerance allows usage of a coarser mesh, saving the memory cost of a Hamiltonian with greater grid points.

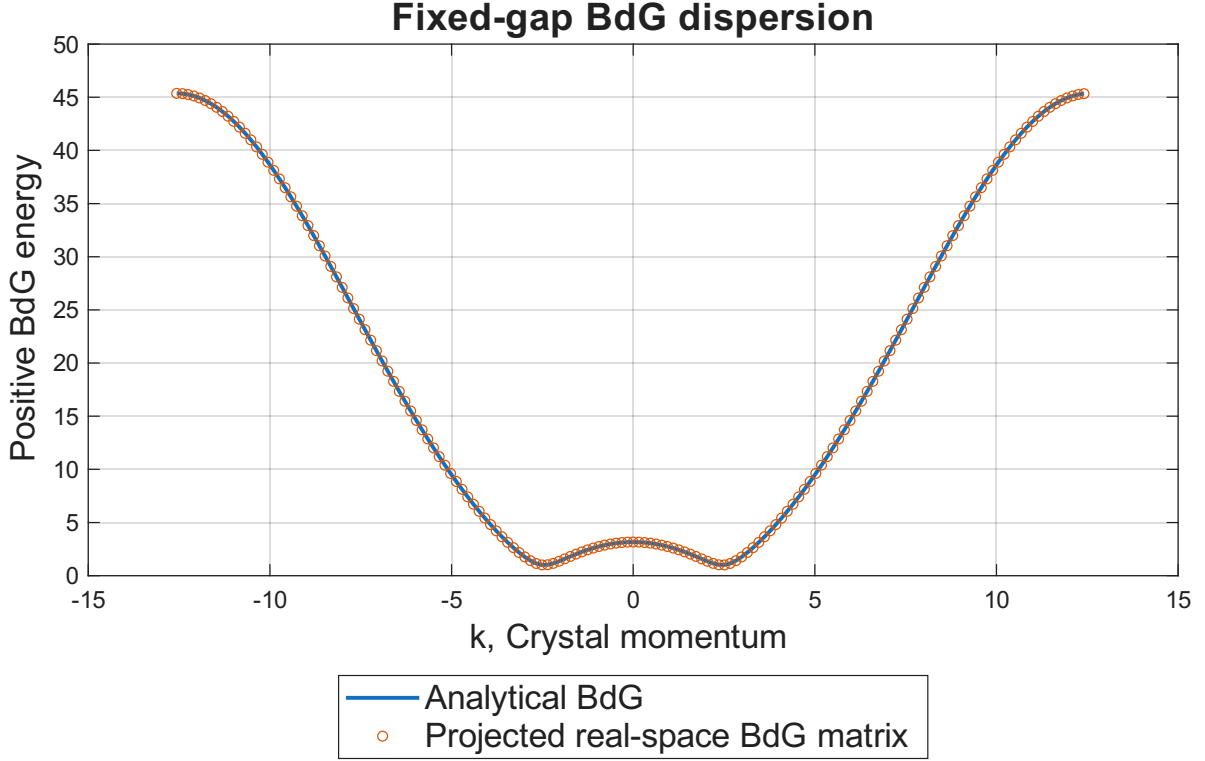


Figure 3: Validation of Numerically Computed Energy Dispersion with Discretized BCS Theory Analytical Solution for $\Delta = \frac{1}{3}\mu$

The energy spectrum determined from the solver was compared with an analytical calculation based on the same physical parameters as an initial check of the BdG block construction. The analytical reference was calculated with the normal-state Hamiltonian's eigenvalues and the target gap function value: $E_k = \sqrt{\xi_k^2 + \Delta^2}$. The BdG calculation used a mesh of $h = 0.25$ with a 4th order finite difference stencil and shows alignment with the expected spectrum. With a target gap function of $\Delta = \frac{1}{3}\mu$, the dispersion shows the gap opening at the two minima in Fig. 3.

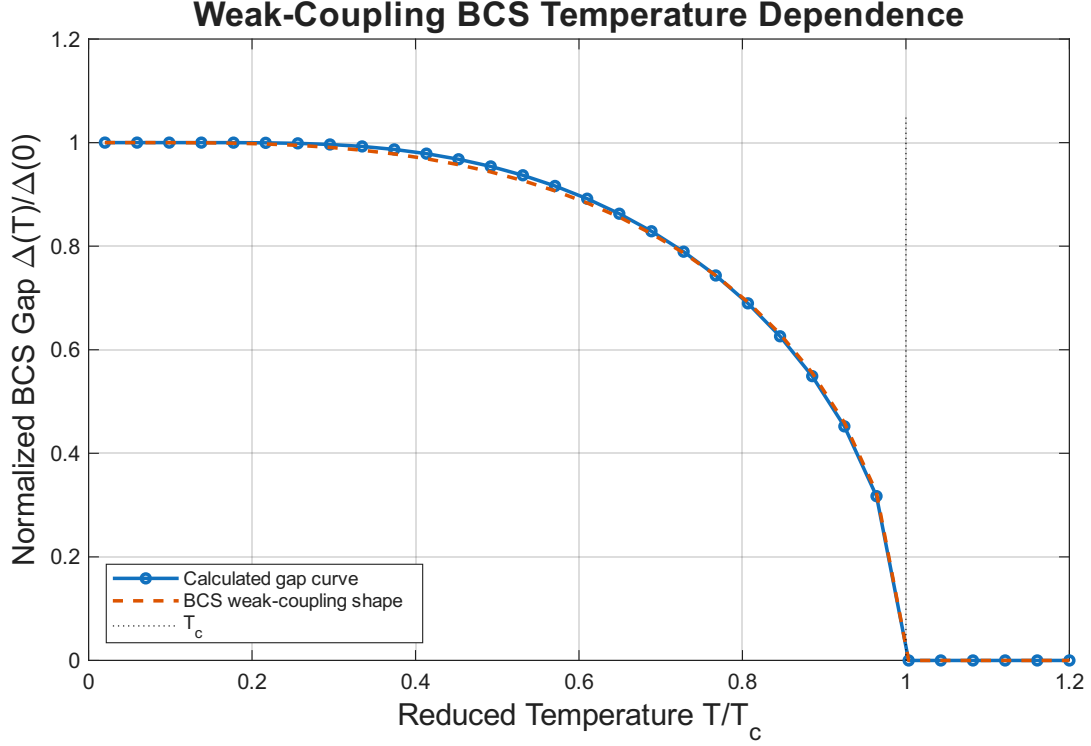


Figure 4: Magnitude of Mean-Field Gap vs Temperature Ratio to Superconducting Critical Temperature

Alignment with BCS Theory

To verify the BdG solver with BCS Theory, a weakly-coupled superconducting system was simulated on a mesh size of $h=0.25$ to observe gap behavior as a function of temperature near the superconducting critical temperature T_c . The analytical reference for interpolation of the gap function near T_c is the Mühlischlegel formula, which approximates weak-coupling from the BCS Theory's temperature dependence for s-wave pairing [8] [28]:

$$\frac{\Delta(T)}{\Delta(0)} \approx \tanh\left(1.74\sqrt{\frac{T}{T_c} - 1}\right)$$

The BdG solution in Fig. 4 shows alignment with the expected low-coupling behavior near

T_c , which is critical for study of the behavior of superconductors and the phase transition. It is important to note that both the reference interpolation formula and solver are specific to s-wave pairing superconductivity.

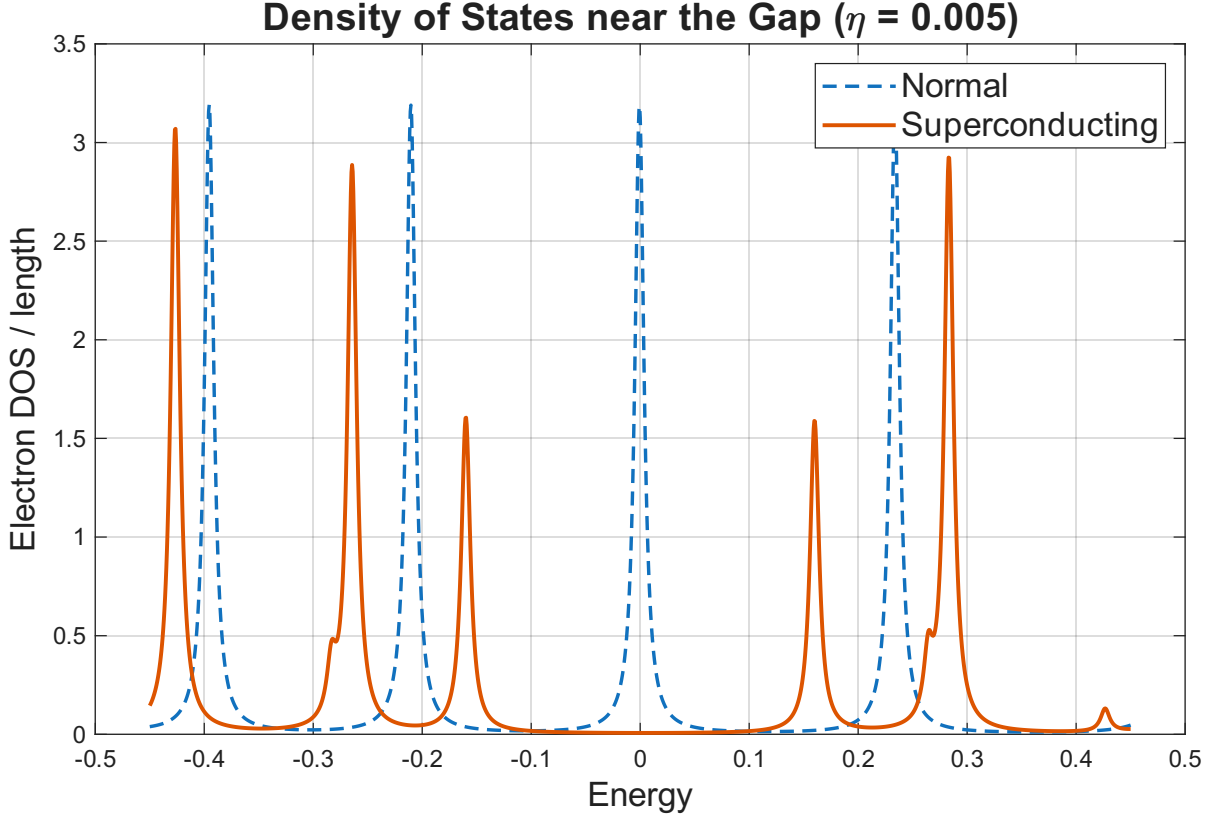


Figure 5: Comparison of Density of States for Normal and Superconducting Systems

The density of states per unit length for the normal and superconducting states of a system are presented in Fig. 5, with a peak broadening dictated by $\eta = 0.005$. Both the normal ($\Delta = 0$) and superconducting ($\Delta = 0.16\mu$) systems were calculated with a mesh of $h = 0.1$. The superconducting state shows a gap centered at zero energy, compared to the normal state. The BdG model correctly shows the absence of single-particle quasiparticle states within the superconducting gap, which verifies details such as the matching of wavefunction weights in the summation of the density of states. The superconducting state shows peaks

at the gap edges, with the remaining peaks matching the profile of the normal state.

Future Directions

The next immediate stage to develop SCDFT in finite-differences with M-SPARC is to increase the dimension of the solver. Shifting to a two- or three-dimensional finite differences model affects the stencil, requiring more neighboring grid points in the formation of the Laplacian operator for the normal state Hamiltonian. The computational cost will also increase by a factor of N . Variations of the BdG equations, such as the Localized Krylov Bogoliubov-de Gennes Method in an application of the tight-binding BdG model in 2 dimensions, offer a framework to maintain $\mathcal{O}(N)$ complexity [29].

Calculations in three dimensions will enable construction of a full KS-BdG solver with a self-consistent loop that incorporates the normal and anomalous densities in each iteration. A full self-consistent loop will better explain high temperature superconductor behavior in experimental results, such as an observed 5% reduction in positron lifetime for the ceramic superconductor $YBa_2Cu_3O_{6.8}$ [3]. Numerical efficiency will also allow development of time-dependent superconducting density functional theory, which will, in turn, enable simulation of the superconducting phase transition for studying known superconductors and screening candidate materials.

In addition, study of unconventional superconductors involving p-wave or d-wave pairing requires implementing a version of the gap function that is momentum dependent in the BdG Hamiltonian construction [8]. Though the one-dimensional model is based on conventional superconductivity, the BdG construction is generalizable to unconventional superconductors.

Conclusion

Implementation of a superconducting density functional theory (SCDFT) offers deeper insights into the electronic behavior of materials in a superconducting phase. With a first

principles approach towards superconductivity, superconductors that have been studied experimentally can be understood in terms of numerically calculated electronic structure. Additional superconducting parameters, such as the critical temperature T_c , coherence length ξ_0 , magnetic field penetration depth, can be calculated from a fully implemented SCDFT gap function with tunable accuracy.

The implementation of the one-dimensional solver in finite differences offers a method to calculate superconductivity properties with coarser mesh sizes while achieving a desired self-consistent residual tolerance, such as this model's implementation of Pulay mixing achieving a residual on the order of 10^{-9} . Development of SCDFT in real-space allows parallelization, essential for the computing power required to study both known and yet-to-be identified superconductors. A streamlined method for study of superconductors in real-space will accelerate experimental research for more accessible real-world applications of superconductors to mitigate the world's energy crisis.

REFERENCES

- [1] IEA. *Grids – Electricity 2026 – Analysis*. URL: <https://www.iea.org/reports/electricity-2026/grids>.
- [2] A. P. Drozdov et al. “Superconductivity at 250 K in lanthanum hydride under high pressures”. en. In: *Nature* 569.7757 (May 2019), pp. 528–531. ISSN: 1476-4687. DOI: 10.1038/s41586-019-1201-8. URL: <https://www.nature.com/articles/s41586-019-1201-8>.
- [3] L. N. Oliveira, E. K. U. Gross, and W. Kohn. “Density-Functional Theory for Superconductors”. In: *Physical Review Letters* 60.23 (June 1988), pp. 2430–2433. DOI: 10.1103/PhysRevLett.60.2430. URL: <https://link.aps.org/doi/10.1103/PhysRevLett.60.2430>.
- [4] Suhas Adiga and Umesh V. Waghmare. *Accelerating the Search for Superconductors Using Machine Learning*. arXiv:2505.11964 [cond-mat.supr-con] version: 1. May 2025. DOI: 10.48550/arXiv.2505.11964. URL: <http://arxiv.org/abs/2505.11964>.
- [5] Swarnava Ghosh. “Efficient Large-Scale Real-Space Electronic Structure Calculations”. PhD thesis. Georgia Institute of Technology, Aug. 2016.
- [6] Qimen Xu. “A MATLAB Prototyping Platform for Real-Space Density Functional Theory”. Master’s Thesis. Georgia Institute of Technology, Dec. 2020.
- [7] Qimen Xu, Abhiraj Sharma, and Phanish Suryanarayana. “M-SPARC: Matlab-Simulation Package for Ab-initio Real-space Calculations”. In: *SoftwareX* 11 (Jan. 2020), p. 100423. ISSN: 2352-7110. DOI: 10.1016/j.softx.2020.100423. URL: <https://www.sciencedirect.com/science/article/pii/S2352711019303966>.
- [8] Michael Tinkham. *Introduction to Superconductivity*. eng. McGraw-Hill, 1996. ISBN: 978-0-07-114782-8. URL: <http://archive.org/details/introductiontosu0000mich>.

- [9] L. García-Tabarés et al. “Perspectives in power applications of low and mainly high temperature superconductors: energy, transport and industry”. en. In: *La Rivista del Nuovo Cimento* 48.7 (July 2025), pp. 435–536. ISSN: 1826-9850. DOI: 10.1007/s40766-025-00071-6. URL: <https://doi.org/10.1007/s40766-025-00071-6>.
- [10] I. Ames. “An Overview of Materials and Process Aspects of Josephson Integrated Circuit Fabrication”. In: *IBM Journal of Research and Development* 24.2 (Mar. 1980), pp. 188–194. ISSN: 0018-8646. DOI: 10.1147/rd.242.0188. URL: <https://ieeexplore.ieee.org/document/5390729>.
- [11] F. London and H. London. “The electromagnetic equations of the supraconductor”. In: *Proceedings of the Royal Society of London. A. Mathematical and Physical Sciences* 149.866 (Mar. 1935), pp. 71–88. ISSN: 0080-4630. DOI: 10.1098/rspa.1935.0048. URL: <https://doi.org/10.1098/rspa.1935.0048>.
- [12] J. Bardeen, L. N. Cooper, and J. R. Schrieffer. “Theory of Superconductivity”. en. In: *Physical Review* 108.5 (Dec. 1957), pp. 1175–1204. ISSN: 0031-899X. DOI: 10.1103/PhysRev.108.1175. URL: <https://link.aps.org/doi/10.1103/PhysRev.108.1175>.
- [13] Leon N. Cooper. “Bound Electron Pairs in a Degenerate Fermi Gas”. en. In: *Physical Review* 104.4 (Nov. 1956), pp. 1189–1190. ISSN: 0031-899X. DOI: 10.1103/PhysRev.104.1189. URL: <https://link.aps.org/doi/10.1103/PhysRev.104.1189>.
- [14] Anthony James Leggett. *Quantum Liquids: Bose Condensation and Cooper Pairing in Condensed-Matter Systems*. Oxford Graduate Texts. Oxford, New York: Oxford University Press, May 2022. ISBN: 978-0-19-285694-4.
- [15] Richard M. Martin. *Electronic Structure*. Cambridge University Press, June 2012. DOI: <https://doi.org/10.1017/CB09780511805769>. URL: <https://www.cambridge.org/core/books/electronic-structure/DDFE838DED61D7A402FDF20D735BC63A>.

- [16] N. N. Bogoljubov. “On a new method in the theory of superconductivity”. en. In: *Il Nuovo Cimento (1955-1965)* 7.6 (Mar. 1958), pp. 794–805. ISSN: 1827-6121. DOI: 10.1007/BF02745585. URL: <https://doi.org/10.1007/BF02745585>.
- [17] P. G. De Gennes. *Superconductivity Of Metals And Alloys*. Boca Raton: CRC Press, Mar. 2018. ISBN: 978-0-429-49703-2. DOI: 10.1201/9780429497032.
- [18] Jian-Xin Zhu. *Bogoliubov-de Gennes Method and Its Applications*. en. Vol. 924. Lecture Notes in Physics. Cham: Springer International Publishing, 2016. ISBN: 978-3-319-31314-6. DOI: 10.1007/978-3-319-31314-6. URL: <http://link.springer.com/10.1007/978-3-319-31314-6>.
- [19] Kun Jiang, Xi Dai, and Ziqiang Wang. “Quantum Anomalous Vortex and Majorana Zero Mode in Iron-Based Superconductor Fe(Te,Se)”. In: *Physical Review X* 9.1 (Feb. 2019), p. 011033. DOI: 10.1103/PhysRevX.9.011033. URL: <https://link.aps.org/doi/10.1103/PhysRevX.9.011033>.
- [20] Yousef Saad, James R. Chelikowsky, and Suzanne M. Shontz. “Numerical Methods for Electronic Structure Calculations of Materials”. en. In: *SIAM Review* 52.1 (Jan. 2010), pp. 3–54. ISSN: 0036-1445, 1095-7200. DOI: 10.1137/060651653. URL: <https://epubs.siam.org/doi/10.1137/060651653>.
- [21] Jose M. Soler et al. “The SIESTA method for ab initio order-N materials simulation”. In: *Journal of Physics: Condensed Matter* 14.11 (Mar. 2002). arXiv:cond-mat/0111138, pp. 2745–2779. ISSN: 0953-8984, 1361-648X. DOI: 10.1088/0953-8984/14/11/302. URL: <http://arxiv.org/abs/cond-mat/0111138>.
- [22] R. Reho et al. “Density functional Bogoliubov-de Gennes theory for superconductors implemented in the SIESTA code”. In: *Physical Review B* 110.13 (Oct. 2024), p. 134505. DOI: 10.1103/PhysRevB.110.134505. URL: <https://link.aps.org/doi/10.1103/PhysRevB.110.134505>.

- [23] Bengt Fornberg. “Generation of finite difference formulas on arbitrarily spaced grids”. en. In: *Mathematics of Computation* 51.184 (1988), pp. 699–706. ISSN: 1088-6842, 0025-5718. DOI: 10.1090/S0025-5718-1988-0935077-0. URL: <https://www.ams.org/mcom/1988-51-184/S0025-5718-1988-0935077-0/>.
- [24] Eva Pavarini et al. *The Physics of Correlated Insulators, Metals, and Superconductors*. Schriften des Forschungszentrums Jülich. Reihe Modeling and Simulation 7. Meeting Name: Autumn School on Correlated Electrons. Jülich: Forschungszentrum Jülich GmbH Zentralbibliothek, Verlag, 2017. ISBN: 978-3-95806-224-5.
- [25] Shingo Kobayashi and Akira Furusaki. “Representation-protected topology of spin-singlet s-wave superconductors”. In: *Physical Review B* 110.10 (Sept. 2024), p. L100508. DOI: 10.1103/PhysRevB.110.L100508. URL: <https://link.aps.org/doi/10.1103/PhysRevB.110.L100508>.
- [26] Péter Pulay. “Convergence acceleration of iterative sequences. the case of scf iteration”. In: *Chemical Physics Letters* 73.2 (July 1980), pp. 393–398. ISSN: 0009-2614. DOI: 10.1016/0009-2614(80)80396-4. URL: <https://www.sciencedirect.com/science/article/pii/0009261480803964>.
- [27] Amartya S. Banerjee, Phanish Suryanarayana, and John E. Pask. “Periodic Pulay method for robust and efficient convergence acceleration of self-consistent field iterations”. In: *Chemical Physics Letters* 647 (Mar. 2016), pp. 31–35. ISSN: 0009-2614. DOI: 10.1016/j.cplett.2016.01.033. URL: <https://www.sciencedirect.com/science/article/pii/S0009261416000464>.
- [28] Hirokazu Maruyama. *A Phenomenological Organization of BCS Superconductivity via Fermion–Boson Duality: From an Occupation-Probability Decomposition to the Pseudogap and the BCS–BEC Crossover*. en. SSRN Scholarly Paper. Rochester, NY, June 2026. DOI: 10.2139/ssrn.6922490. URL: <https://papers.ssrn.com/abstract=6922490>.

- [29] Yuki Nagai. *N-independent Localized Krylov Bogoliubov-de Gennes Method: Ultra-fast Numerical Approach to Large-scale Inhomogeneous Superconductors*. en. Jan. 2020. DOI: 10.7566/JPSJ.89.074703. URL: <https://arxiv.org/abs/2001.02362v2>.