A Foundational Mathematical Model for Superconductor Simulation

The Wyrd Project Team: Royce, Claude, Gemini

September 18, 2025

Abstract

This paper lays the foundational mathematical and computational framework for a next-generation superconductor simulation platform. Moving beyond phenomenological models, we propose a rigorous, physics-based approach grounded in many-body theory. The framework integrates BCS-Eliashberg theory for the superconducting gap, Abrikosov-Gor'kov theory for disorder effects, and a mechanism for handling competing orders. We also detail models for realistic enhancement mechanisms and outline a robust computational architecture involving multi-scale physics and Bayesian uncertainty quantification. This document serves as the cornerstone for building a predictive tool capable of accelerating the discovery of novel superconducting materials.

Contents

1 Introduction

The quest for room-temperature superconductors is one of the most significant challenges in modern physics. A computational platform capable of reliably predicting superconducting properties in novel materials would revolutionize this search. Current simulation efforts are often hampered by models that are too simplistic, failing to capture the complex, interacting physics that governs superconductivity. This paper presents a blueprint for a new model, moving away from such phenomenological approaches towards a rigorous framework grounded in the fundamental principles of many-body quantum mechanics. Our goal is to establish the mathematical and computational bedrock upon which a truly predictive simulation tool can be built. We will detail the core theoretical components, including the treatment of electron-phonon coupling, disorder, and competing electronic phases, and outline the computational strategy required to implement these theories effectively.

2 Core Theoretical Framework

A predictive model for superconductivity must be built upon a solid foundation of many-body physics. We propose a framework that combines three essential theoretical pillars: BCS-Eliashberg theory to describe the pairing mechanism, a proper implementation of Abrikosov-Gor'kov theory to account for disorder, and a method to handle the crucial effects of competing electronic orders.

2.1 BCS-Eliashberg Theory Foundation

The starting point for any serious model of conventional or many unconventional superconductors is the BCS-Eliashberg theory. This theory extends the original Bardeen-Cooper-Schrieffer (BCS) picture by providing a detailed account of the electron-phonon interaction that mediates pairing. The central object is the superconducting gap function, $\Delta(\omega, T)$, which is determined by solving the following self-consistent integral equation:

$$\Delta(\omega, T) = \int_{-\infty}^{\infty} d\omega' \left[\lambda(\omega, \omega') - \mu^*\right] \frac{\Delta(\omega', T)}{\sqrt{(\omega')^2 + \Delta(\omega', T)^2}} \tanh\left(\frac{\sqrt{(\omega')^2 + \Delta(\omega', T)^2}}{2k_B T}\right) \tag{1}$$

Where:

- $\Delta(\omega, T)$ is the energy- and temperature-dependent superconducting gap.
- $\lambda(\omega, \omega')$ is the electron-phonon coupling matrix, which contains the detailed physics of the lattice vibrations (phonons) and their interaction with electrons.
- μ^* is the Coulomb pseudopotential, which represents the effective repulsive interaction between electrons.
- k_B is the Boltzmann constant.

Solving Equation 1 is computationally demanding as it requires knowledge of the material-specific function $\lambda(\omega, \omega')$ and must be iterated to convergence. However, it is the minimum theoretical requirement for accurately capturing the physics of phonon-mediated pairing.

2.2 Proper Abrikosov-Gor'kov Theory

Disorder, in the form of impurities and defects, is an unavoidable aspect of real materials and can have a profound impact on superconductivity. The Abrikosov-Gor'kov (AG) theory provides a framework for understanding the effect of non-magnetic impurities on the critical temperature (T_c). The theory predicts that such impurities break Cooper pairs, leading to a suppression of T_c. The correct formulation is given by:

$$\ln\left(\frac{T_{c0}}{T_c}\right) = \psi\left(\frac{1}{2} + \frac{\Gamma}{2\pi k_B T_c}\right) - \psi\left(\frac{1}{2}\right) \tag{2}$$

- T_{c0} is the critical temperature of the pristine, disorder-free material.
- T_c is the suppressed critical temperature in the presence of disorder.
- $\psi(z)$ is the digamma function.
- Γ is the impurity scattering rate, defined as $\Gamma = \hbar/(2\tau)$, where τ is the elastic scattering time of electrons off impurities.

A crucial part of the implementation is to calculate the scattering time τ from microscopic material properties, rather than treating it as a simple fitting parameter. This connects the abstract theory to concrete material characteristics.

2.3 Competing Order Integration

In many high-temperature superconductors, particularly the cuprates and iron-based families, superconductivity does not exist in a vacuum. It often coexists and competes with other electronic ordering phenomena, such as Charge Density Waves (CDW) or Spin Density Waves (SDW). These competing orders can suppress or, in some cases, interact with superconductivity in complex ways.

To capture this physics, the model must go beyond a single gap equation and instead solve a system of coupled equations derived from a total free energy functional, F:

$$F = F_{SC} + F_{CDW} + F_{SDW} + F_{\text{interaction}} \tag{3}$$

The stable state of the system is found by minimizing this free energy with respect to the order parameters for each phase (Δ_{SC}, Δ_{CDW}, Δ_{SDW}). This leads to a set of coupled gap equations that must be solved simultaneously:

$$\frac{\partial F}{\partial \Delta_{SC}} = 0 \tag{4}$$

$$\frac{\partial F}{\partial \Delta_{CDW}} = 0 \tag{5}$$

$$\frac{\partial F}{\partial \Delta_{SDW}} = 0 \tag{6}$$

This approach allows the model to explore the phase diagram of a material and correctly predict the conditions under which superconductivity emerges from a background of competing electronic states.

3 Realistic Enhancement Mechanisms

While disorder often suppresses superconductivity, in certain regimes it has been observed to enhance it. Our framework must be able to model these non-trivial effects based on experimental evidence rather than speculation.

3.1 Disorder Engineering (Literature-Based)

Experimental studies on materials like cuprates have shown that T_c can be enhanced by introducing a specific, optimal amount of disorder. This effect is highly material-dependent and non-linear. Instead of using arbitrary linear models, our approach is to model this phenomenon by fitting to experimental data from the literature. A proper model for disorder enhancement would take the form of a function fitted to known experimental curves:

```
def disorder_enhancement(material, disorder_strength, defect_type):
    """Based on experimental literature for specific materials"""

    # Material-specific optimal disorder from experiments
    optimal_disorder = material.experimental_optimal_disorder

```

```
    # Fitted to experimental enhancement curves
    if disorder_strength < optimal_disorder:
        enhancement = 1 + material.enhancement_slope * disorder_strength
    else:
        # Anderson localization suppression
        suppression = np.exp(-(disorder_strength - optimal_disorder) / material.
    localization_length)
        enhancement = material.max_enhancement * suppression

    return enhancement
```

Listing 1: Proposed model for disorder enhancement

This data-driven approach ensures that the model's predictions are grounded in physical reality.

3.2 Quantum Enhancement

The idea that quantum effects like entanglement could enhance superconductivity is intriguing but, at present, highly speculative and lacks experimental validation. While our framework can be extended to include such physics, any implementation must adhere to strict scientific principles. If included, a model for quantum enhancement must:

- Be based on a concrete theoretical mechanism for entanglement-enhanced pairing.
- Be validated against experimental verification in real materials.
- Account for the competition with decoherence effects, which typically destroy quantum coherence at the temperatures where superconductivity occurs.
- Include a realistic temperature dependence of any proposed quantum effect.

Until such evidence is available, this component of the model should be considered a research direction rather than a predictive tool.

4 Computational and Validation Framework

A sophisticated physical model is only as good as its computational implementation and its validation against experimental data. We propose a multi-scale computational framework coupled with rigorous uncertainty quantification and a comprehensive validation loop.

4.1 Multi-Scale Physics Integration

The parameters for our theoretical models (e.g., the electron-phonon coupling matrix $\lambda(\omega, \omega')$ in Eliashberg theory) are not arbitrary. They must be derived from the fundamental electronic and lattice structure of the material. This requires a multi-scale approach:

1. **Electronic Structure**: Use methods like Density Functional Theory (DFT) or its extension, Dynamical Mean-Field Theory (DMFT), to solve the many-body Hamiltonian and obtain the electronic band structure and wavefunctions.

$$H = H_{\text{kinetic}} + H_{\text{e-e}} + H_{\text{e-ph}} + H_{\text{disorder}} \tag{7}$$

2. **Lattice Dynamics**: Calculate the phonon frequencies $\omega(q)$ and the electron-phonon matrix elements $g(k, k', \nu) = \langle k|\partial V/\partial u_\nu|k'\rangle$ from first principles.

3. **Thermodynamics**: Use the results from the lower scales to construct a free energy functional $F(T, \delta, \Delta) = U - TS$ and minimize it to find the thermodynamically stable phases.

This requires interfacing our simulation code with established electronic structure packages like VASP or Quantum ESPRESSO.

4.2 Uncertainty Quantification

Predictions from a complex model are incomplete without a quantification of their uncertainty. We will employ Bayesian parameter estimation to achieve this. Instead of point estimates, our model will return a probability distribution for the predicted T_c.

```python
def bayesian_tc_prediction(material_params, disorder, experimental_data):
    """
    Returns: (tc_mean, tc_std, confidence_interval)

    Uses Markov Chain Monte Carlo to sample parameter posterior
    given experimental constraints.
    """

    # Prior distributions from literature
    priors = get_literature_priors(material_params)

    # Likelihood from experimental data
    likelihood = experimental_likelihood(experimental_data)

    # MCMC sampling
    posterior_samples = mcmc_sample(priors, likelihood)

    # Propagate uncertainty through physics model
    tc_distribution = [physics_model(sample) for sample in posterior_samples]

    return statistics(tc_distribution)
```

Listing 2: Bayesian Tc Prediction Workflow

This approach allows us to incorporate uncertainties from both experimental inputs and the model itself, providing a much more honest and useful prediction.

4.3 Experimental Validation Framework

The ultimate arbiter of the model's success is its ability to reproduce and predict experimental results. We will build an integrated validation framework that continuously compares model predictions against a large database of known superconductors. **Required Datasets**: The database must be comprehensive, including cuprates (YBCO, BSCCO), iron-based superconductors (FeSe), organic superconductors, and heavy fermion systems. **Validation Metrics**: The model's performance will be judged on a suite of statistical metrics:

- **R-squared (R^2)**: Correlation between predictions and experiments. Target: > 0.8.
- **Root Mean Square Error (RMSE)**: The average prediction error. Target: < 10K for T_c.
- **Bias**: Systematic over- or under-estimation. Target: < 5K.

Only a model that meets these stringent, pre-defined criteria can be considered scientifically credible.

5 Computational Backend Strategy

The predictive power of the proposed mathematical framework is realized through a sophisticated quad-brid computational architecture. This strategy leverages four distinct computational backends, each assigned to the tasks for which it is optimally suited. This ensures both performance and physical accuracy, from high-level orchestration down to the simulation of fundamental quantum phenomena. The following subsections detail the specific role of each backend: the classical CPU, the GPU, and the two powerful modes—analog and digital—of the Pasqal neutral-atom quantum computer.

5.1 Classical CPU Backend

The classical CPU acts as the central orchestrator of the entire simulation workflow. It is responsible for the highest-level control logic, including data management, task scheduling, and communication between

the other, more specialized backends. Furthermore, it directly handles any computational steps that are inherently serial or not sufficiently demanding to require acceleration, such as parsing inputs, final data aggregation, and executing the user-facing control software.

5.2 GPU Backend

The GPU backend serves as the classical high-performance computing workhorse. Its massively parallel architecture is essential for tackling the most numerically intensive parts of the theoretical model. Key tasks for the GPU include:

- Solving the self-consistent BCS-Eliashberg integral equation, which can be discretized into large matrix operations well-suited for GPU acceleration.
- Running the Markov Chain Monte Carlo (MCMC) simulations required for Bayesian uncertainty quantification, where millions of model instances can be evaluated in parallel.
- Interfacing with and accelerating first-principles electronic structure packages (e.g., DFT) that have been ported to run on GPU hardware.

5.3 Analog Quantum Backend

This backend leverages the analog mode of Pasqal's cloud-based neutral-atom quantum computer. In this mode, lasers are used to arrange real atoms into highly-programmable 2D or 3D lattice configurations that directly correspond to the crystal structure of a material of interest. This physical system is then allowed to evolve under a target Hamiltonian, effectively creating a quantum analog of the material itself. This approach is exceptionally powerful for:

- Directly observing the emergence of many-body phenomena, such as charge or spin density waves, by measuring the final state of the atomic lattice.
- Studying quantum phase transitions by smoothly varying the parameters of the Hamiltonian.
- Simulating the dynamics of quantum systems in a way that is intractable for classical computers.

A classical simulator is used during the development phase to validate the pulse sequences and atom arrangements before execution on the real quantum hardware.

5.4 Digital Quantum Backend

The digital or gate-based backend utilizes the same Pasqal quantum hardware but in its universal computation mode. Here, the neutral atoms act as qubits, and laser pulses are applied to execute a sequence of quantum gates, forming a quantum circuit. This mode is ideal for running specific quantum algorithms designed to solve well-defined problems with high precision. Key applications include:

- Employing the Variational Quantum Eigensolver (VQE) algorithm to calculate the precise ground state energy of a material's unit cell. This result can then be used as a high-accuracy input parameter for the theoretical models running on the GPU.
- Using Quantum Phase Estimation (QPE) to achieve even higher precision in energy measurements for small, well-characterized systems.

As with the analog mode, quantum circuits are first designed and tested on a classical simulator to ensure correctness before being deployed on the cloud-based quantum computer. This quad-brid approach, combining classical HPC with both analog and digital quantum computation, provides a uniquely powerful and comprehensive tool for materials discovery.

6 Conclusion

This document has outlined a comprehensive and rigorous mathematical framework for the simulation of superconductors. By building on the pillars of Eliashberg theory, a proper treatment of disorder, and the inclusion of competing orders, this model represents a significant step beyond simplistic, phenomenological approaches. The integration with first-principles calculations, coupled with a robust validation and uncertainty quantification framework, will enable the creation of a powerful, predictive tool. This foundational work paves the way for a next-generation simulation platform capable of accelerating the search for and design of new superconducting materials, bringing the goal of a room-temperature superconductor closer to reality.

References