In order to effectively model and potentially predict superconductivity within a given material be it a conventional superconductor, unconventional superconductor, topological superconductor, or any other form of material, a comprehensive theory describing the microscopic interactions between atoms and other microscopic particles comprising said material along with their effects on the superconducting state must by necessity be created. The currently utilized BCS theory is in its current form not viable as a result of its incorrect conjecture that a phonon interaction mechanism (lattice vibration based mechanism) directly leads to the condensation of cooper electron pairs. This mechanism has been primarily disproven by the frequent updates or as JE Hirsch specifies “increases made to the value of the electron-phonon coupling constant.” This somewhat indirectly shows that it's not the phonon electron coupling constant or even a phonon effect that contributes to the condensation of cooper pairs but something else that has a direct effect on lattice vibration (phonons are quasiparticles used to describe lattice vibration within a superconductor). Despite that fundamental flaw, JE Hirsch states that BCS theory presents a number of indisputable proven facts such as the cooper electron pairing concept, the existence of macroscopic phase coherence, and the notion of the existence of an energy gap. In the process of describing a new theory for superconductivity these ideas would necessarily have to be included.

In order to expediently construct such a theory a number of BCS theory’s derivations can (and have to) be reused albeit heavily modified in order to create a new more comprehensive theory. This theory will be based off of a modified/reworked version of the London equations, instead of utilizing the Drude model/theory of conductivity which was a classical physics based approach to modelling electron behaviour developed in 1900, the London equations will be redeveloped from a quantum mechanics based theory of conductivity (or more specifically electron interaction), for this study Quantum Electrodynamics theory will be used. Additionally an effort will be made to formally derive these new London equations where possible as the original London equations are derived through intuitive logic which can be prone to unique errors as many systems such as quantum mechanics based systems and even some classical systems with chaos as an element tend to behave in ways “intuitive logic” or even intuition itself (in the case of quantum systems) cannot predict. Following that the major aspects of BCS theory will be rederived in order to create a basic framework descending from quantum mechanics, that describes the superconducting state, this will serve as the basis for this attempt at a comprehensive theory of superconductivity. This process is unfortunately complicated by the heavy reliance Bardeen, Cooper and Schrieffer placed on the classical kinetic interpretation of electron interactions. Building upon the preliminary framework that will be created it is necessary to describe the cooper pairing mechanism through a novel non-phonon/non-lattice vibration mechanism. Once that aspect of the study is completed the resulting equations can be converted into a gapped Hamiltonian system. This process makes the equations easier to work with which will enable them to be used to model and evaluate superconductor systems.

Calculating or modelling any substantial or statistically significant superconducting system would be highly impractical using “paper and pencil” calculations, as such the theory/Hamiltonian would have to be incorporated into a computer simulation suite of some sort in order to hasten the process. Density Functional Theory is the “most popular and among the most successful approaches” to modelling the electronic structure of many body systems, as the phenomenon being modelled is partially electric in nature this modelling approach would be one of the best approaches to use in order to predict the properties of superconducting materials, however there also exists a “Superconducting Density Functional Theory” which may be used instead of plain DFT in order to further hasten progress by easing the necessary workload. Additionally molecular dynamics simulations will be used in conjunction with the DFT or SCDFT simulations to form the complete (for the scope of this study) model of the superconductor being simulated. The molecular dynamics simulation in particular will help define/predict a given superconductors physical parameters/

Once the simulation/modelling suite is complete, the suite will be installed within systems running arch linux in order to utilization computational resources with the most possible efficiency. From there data can be collected on the electrical interactions within the simulation. To do so a few unit cells of a given material will be simulated (as 1 unit cell may lead to unintended/undesired effects emerging and or it may also lead to some effects being simulated poorly). To be more specific, currently a cubic model of 27 unit cells will be modelled/simulated. This number has been selected so as to minimize the time a simulation of a given superconducting system will take while also ensuring that the simulation is accurate within at least a few of the inner unit cells. Currently it is expected that parameters/effects such as magnetic response, magnetic flux density, temperature variation of electrical resistivity, electron speed, molecular vibration, upper critical field, lower critical field, London penetration depth, coherence length, critical current density and band gap, will be collected. Additionally should additional relevant parameters become identified prior to the start of simulation operations they will be added to this list, once simulation/data collection starts no changes to the scope of this study will be made. Each superconducting material will be simulated at least twice, with the data between both runs being compared to ensure no random error has occurred. For the first 10-25 runs of the simulation suite the superconductors being studied will be conventional superconductors. The parameters collected on those simulated superconductors will then be compared to at least 2 publicly available sources (per superconductor) that physically analyze said superconducting material (that is to say studies that solely measure the parameters and or mathematically calculate some parameters based off of physically collected data), if the simulated parameters match the measured parameters within an error margin of +10% -5% (to accommodate for error) the mathematical model of superconductivity being constructed by this study will be considered in parity with at least BCS theory. From there simulation/modelling attempts can begin for unconventional superconductors. The same process will be applied to unconventional superconductors as was applied to the conventional superconductors, parameters will be collected and compared to publicly available data. If even a few simulated unconventional superconductor parameters are in parity with the actual observed values then the theory will be considered to be at the least a semi accurate model of superconductivity and a significant step forward in superconducting theory. Should the calculated parameters of all of the unconventional superconductor material families be accurately (within the margin of error) modelled/simulated then the theory developed here can be considered completely in parity with reality and the goal of this study will be more than achieved.