# Computer Modeling of P-wave Superconductivity

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# Brief History

- Superconductivity was first discovered in 1911 by the Dutch physicist Heike Kamerlingh Onnes of Leiden University
- Noticed that if pure Mercury was cooled to below certain temperatures, all electrical resistance disappeared
- Sparked an interest to develop other compounds with the same characteristics

# Magnetic Effects on Compounds

- Noticed that if an external magnetic field were introduced near the superconductor, the induced current would flow in such a way as to mirror the exact field that would have otherwise penetrated the superconductor
- The resulting magnetic force is strong enough to allow a magnet to levitate above the compound

# Critical Temperature

- Critical temperature is the point when a superconducting compound becomes a superconductor at or below that temperature
- Most 20$^{th}$ century research was centered around discovering compounds with high critical temperatures ($T_c$)
- The current record for highest $T_c$ is 138 K

# Hubbard Model

- Electrons on a lattice
- Discrete sites for electrons to occupy
- Periodic boundary conditions; the last point on the lattice structure is connected to the first

- Analyzing the probabilities of the electrons “hopping” from one site to the next is done by analyzing the Hamiltonian Matrix

- For the one dimensional case, the (nonzero) off diagonal elements represent the probability that an electron will jump to an adjacent site

- The evaluation of the eigenvalues of the Hamiltonian allowed for the calculation of the energies and the resultant non-interacting wave functions

- Classically, the diagonal element $A_{jj}$ of the Hamiltonian represent the potential energy at site *j*, which is usually set to zero when each site is equivalent

# Electron Interactions

- These equations are only valid when there is no interaction between electrons of nearby sites
- The interaction parameter (U) describes the Coulomb repulsion between the electrons
- This creates the need for approximations since a many body problem is impossible to solve analytically

# Dynamic Cluster Approximation

- Takes points on a fine grid structure and groups them into points on a coarse grain grid
- Takes the average of the nearest points on the fine grid to calculate each point on the coarse grid
- Enables the analysis of the many body problem (approximately)

# Green's Function Matrices

- The code uses a random number generator to initialize a random pair wave function as a function of electron spin and coordinates
- We then Fourier Transform this into a function of frequency and momentum, as a necessary input to start the calculations

- The Green’s function matrix is then calculated from the dynamic cluster approximation

- This resulting matrix is then used to calculate the self energy of the system

- The first order self energy is obtained by analyzing specific elements of the Green’s function matrix and multiplying them by the interaction U

# More About Self Energy and the Fea

- The infinite order self energy is next evaluated
- Is done through a process known as the fluctuation exchange approximation (fea)
- The Green's function matrices are used to develop what are known as the Chi arrays; linear combinations of the $t < 0$ and $t > 0$ Green's function matrices

- These chi arrays are then Fourier transformed into functions of frequency and momentum

- We use these transformed chi matrices to calculate the sigma (self energy) arrays, and then Fourier Transform them into functions of momentum, which then describe the infinite order self energy

- The first and infinite order energies are then temporarily saved, and the pair wave function, having been changed slightly, is transformed back into a function of spin and coordinates
- The pair wave function is then Fourier transformed back into a function of frequency and momentum, and new Green's function matrices are derived from this new wave function, and the entire process repeats itself

- The new first and infinite order self energies are then compared to the previously calculated energies
- The goal of this process is to have the self energies become exactly the same – such a process is called self consistent

# Chemical Potential of the System

- Once the self energies have converged, the density of electrons per site is calculated as dictated by the chemical potential of the system

- If the calculated density matches the desired density as given from an input file, the iteration loop breaks.  If not, then the chemical potential changes slightly and the whole process starts over

# Symmetry Analysis

- Once the self energies have converged and the density is as desired, the final process is to analyze the symmetry of the system
- The initial pair wave function is random, but as it iterates through the main loop of the program it changes slightly in such a way as to produce an internal symmetry of electron pairs

# Pairing States

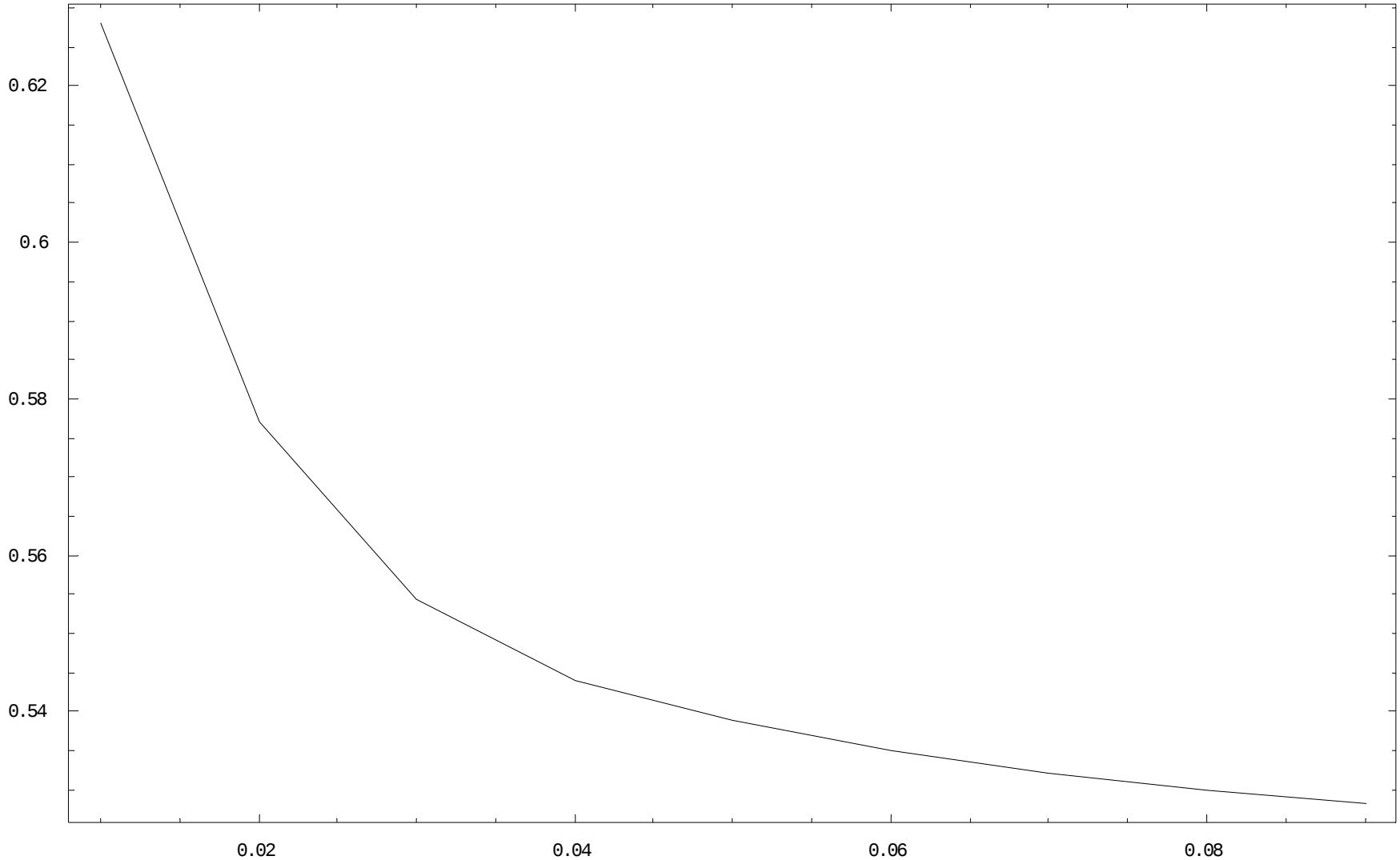
- The parameter that simulates the overall interactions between the electrons is known as the pairing field
- This trick allows the electrons to stick together such that they travel in pairs along the lattice
- This mimics the observed pairing of electrons in superconducting compounds
- After each iteration, the pairing state is recalculated and fluctuates until the desired pairing state is achieve in order to minimize the energy of the system

# Eigenvalues

- The eigenvalues of the converged chi arrays typically are close to 1 (around 0.95) for the system to display superconducting properties

- P-wave superconductivity is theorized to be produced around densities of between 0.4 and 0.6 electrons per site, and as is apparent, will only be possible at very low temperatures

Interaction = 4, Density = 4, Eigenvalue vs Temperature



# Future Work

- Future development of the code will include the calculation of the $2^{nd}$ and $3^{rd}$ order self energies

- Other input parameters such as a magnetic field and a threaded flux will also be taken into consideration