Superconductivity in the attractive Hubbard model in the presence of spin-orbit coupling

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Outline

1. Spin-Orbit coupling in a 2D tight binding model
2. Attractive Hubbard model with spin-orbit coupling
3. Analysis
4. Further directions

Section 1

Spin-Orbit coupling in a 2D tight binding model

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We include the effect of the spin-flipping of an electron while hopping between sites through the following **Spin-Orbit coupling** terms

$$V_{SO} = i \sum_{j,\alpha,\beta} [c^{\dagger}_{j,\alpha} (V_1)_{\alpha\beta}\, c_{j+y,\beta} - c^{\dagger}_{j,\alpha} (V_2)_{\alpha\beta}\, c_{j+x,\beta} - \text{h.c.}] \tag{1}$$

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where,

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$$V_2 = V_R \sigma_y - V_D \sigma_x \tag{3}$$

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The total Hamiltonian is given by

$$H_{SO} = -t \sum_{\langle i,j \rangle, s} (c^{\dagger}_{i,s} c_{j,s} + \text{h.c.}) + V_{SO} \tag{4}$$

Digonalising the Hamiltonian

The Hamiltonian matrix expressed in the momentum basis is given by

$$\begin{pmatrix} c_{k\uparrow}^\dagger & c_{k\downarrow}^\dagger \end{pmatrix} \begin{pmatrix} -2t(\cos k_x + \cos k_y) & 2(S_1 + iS_2) \\ 2(S_1 - iS_2) & -2t(\cos k_x + \cos k_y) \end{pmatrix} \begin{pmatrix} c_{k\uparrow} \\ c_{k\downarrow} \end{pmatrix} \tag{5}$$

where

$$S_1 \equiv V_R \sin(k_y) + V_D \sin(k_x) \tag{6}$$

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The dispersion relation:

$$\epsilon_{k,\pm} = -2t(\cos k_x + \cos k_y) \pm 2\sqrt{S_1^2 + S_2^2} \tag{8}$$

Section 2

Attractive Hubbard model with spin-orbit coupling

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We use the mean field approximation through the pairing channel, under which we can rewrite the Hamiltonian as

$$H = H_{SO} - U \sum_i [\Delta_i c^\dagger_{i\uparrow} c^\dagger_{i\downarrow} + \Delta^*_i c_{i\downarrow} c_{i\uparrow} - |\Delta_i|^2] \tag{10}$$

where $\Delta_i = \langle c_{i\downarrow} c_{i\uparrow} \rangle$ and $\Delta^*_i = \langle c^\dagger_{i\uparrow} c^\dagger_{i\downarrow} \rangle$.

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where $\Delta_i = \langle c_{i\downarrow} c_{i\uparrow} \rangle$ and $\Delta^*_i = \langle c^\dagger_{i\uparrow} c^\dagger_{i\downarrow} \rangle$.
We assume site independent mean-field parameter: $\Delta_i \equiv \Delta$

Hamiltonian matrix in the momentum basis

Once we go to the Fourier space as usual, we get a 4×4 block diagonal form for the Hamiltonian matrix as follows (after doubling up)

$$\begin{pmatrix} c^\dagger_{k\uparrow} & c_{-k\downarrow} & c^\dagger_{k\downarrow} & c_{-k\uparrow} \end{pmatrix}$$
$$\begin{pmatrix} \epsilon^0_k - \mu & -U\Delta & 2(S_1 + iS_2) & 0 \\ -U\Delta^* & -(\epsilon^0_k - \mu) & 0 & 2(S_1 + iS_2) \\ 2(S_1 - iS_2) & 0 & \epsilon^0_k - \mu & U\Delta \\ 0 & 2(S_1 - iS_2) & U\Delta^* & -(\epsilon^0_k - \mu) \end{pmatrix} \begin{pmatrix} c_{k\uparrow} \\ c^\dagger_{-k\downarrow} \\ c_{k\downarrow} \\ c^\dagger_{-k\uparrow} \end{pmatrix} \tag{11}$$

where $\epsilon^0_k = -2t[\cos(k_x) + \cos(k_y)]$

Eigenvalues

Once we diagonalize this matrix, we get the following eigenvalues

$$E^{+}_{k,\pm} = \pm\sqrt{(\epsilon_{k,+} - \mu)^2 + U^2|\Delta|^2} \tag{12}$$

$$E^{-}_{k,\pm} = \pm\sqrt{(\epsilon_{k,-} - \mu)^2 + U^2|\Delta|^2} \tag{13}$$

Eigenvectors

With eigenvectors given by:

$$X^{+}_{k,+} = \frac{1}{2\sqrt{E^{+}_{k}(E^{+}_{k} - (\epsilon_{k,+} - \mu))}} \begin{pmatrix} U\Delta\frac{S_1+iS_2}{\sqrt{S_1^2+S_2^2}} \\ -\frac{S_1+iS_2}{\sqrt{S_1^2+S_2^2}}(E^{+}_{k} - (\epsilon_{k,+} - \mu)) \\ U\Delta \\ E^{+}_{k} - (\epsilon_{k,+} - \mu) \end{pmatrix} \tag{14}$$

$$X^{+}_{k,-} = \frac{1}{2\sqrt{E^{+}_{k}(E^{+}_{k} - (\epsilon_{k,+} - \mu))}} \begin{pmatrix} E^{+}_{k} - (\epsilon_{k,+} - \mu) \\ U\Delta^{*} \\ \frac{S_1-iS_2}{\sqrt{S_1^2+S_2^2}}(E^{+}_{k} - (\epsilon_{k,+} - \mu)) \\ U\Delta^{*}\frac{-S_1+iS_2}{\sqrt{S_1^2+S_2^2}} \end{pmatrix} \tag{15}$$

Eigenvectors

$$X^-_{k,+} = \frac{1}{2\sqrt{E^-_k(E^-_k - (\epsilon_{k,-} - \mu))}} \begin{pmatrix} -U\Delta\frac{S_1+iS_2}{\sqrt{S_1^2+S_2^2}} \\ \frac{S_1+iS_2}{\sqrt{S_1^2+S_2^2}}(E^-_k - (\epsilon_{k,-} - \mu)) \\ U\Delta \\ E^-_k - (\epsilon_{k,-} - \mu) \end{pmatrix} \quad (16)$$

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Ladder operators for the quasi-particles

The BdG transformation is given by

$$\begin{pmatrix} c_{k\uparrow} \\ c^{\dagger}_{-k\downarrow} \\ c_{k\downarrow} \\ c^{\dagger}_{-k\uparrow} \end{pmatrix} = \begin{pmatrix} X^{+}_{k,+} & X^{-}_{k,-} & X^{-}_{k,+} & X^{+}_{k,-} \end{pmatrix} \begin{pmatrix} \gamma_{k\uparrow} \\ \gamma^{\dagger}_{-k\downarrow} \\ \gamma_{k\downarrow} \\ \gamma^{\dagger}_{-k\uparrow} \end{pmatrix} \tag{18}$$

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The Hamiltonian in the the γ basis is given by

$$H = NU|\Delta|^2 \sum_k E^+_k \gamma^\dagger_{k\uparrow}\gamma_{k\uparrow} + E^-_k \gamma^\dagger_{k\downarrow}\gamma_{k\downarrow} - \frac{E^+_k + E^-_k - \epsilon^+_k - \epsilon^-_k}{2} \tag{19}$$

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which is diagonalised as expected.
Therefore, the thermal expectation value of $\gamma^{\dagger}_{k\uparrow}\gamma_{k\uparrow}$ and $\gamma^{\dagger}_{k\downarrow}\gamma_{k\downarrow}$ are

$$\langle \gamma^{\dagger}_{k\uparrow}\gamma_{k\uparrow} \rangle_T = n_F^T(E_k^+) \qquad \langle \gamma^{\dagger}_{k\downarrow}\gamma_{k\downarrow} \rangle_T = n_F^T(E_k^-) \tag{20}$$

Self-consistency of the mean field parameter

The site-independent mean field parameter can be calculated for a thermal state of temperature T

$$\Delta = \frac{1}{N}\sum_i \langle c_{i\downarrow} c_{i\uparrow}\rangle_T = \frac{1}{N}\sum_k \langle c_{-k\downarrow} c_{k\uparrow}\rangle_T \tag{21}$$

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We can use the BdG transformation Eq. (18) and the thermal expectations Eq. (20) to find

$$\Delta = \frac{U\Delta}{4N}\sum_k \frac{1}{E_k^+}\tanh\left(\frac{\beta(E_k^+ - \mu)}{2}\right) + \frac{1}{E_k^-}\tanh\left(\frac{\beta(E_k^- - \mu)}{2}\right) \tag{22}$$

Solve for Δ numerically!

Section 3

Analysis

Analysis

Numerical Methods:

- Fixed Point Acceleration

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- Root finding through Bisection method

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- Fixed Point Acceleration
- Root finding through Bisection method
- Gradient Descent

We find delta for varying parameters, using the above mentioned methods through self consistency and optimisation.

Analysis: Self Consistency

Our self-consistency equation is of the form;

$$\Delta = f(\Delta) \tag{23}$$

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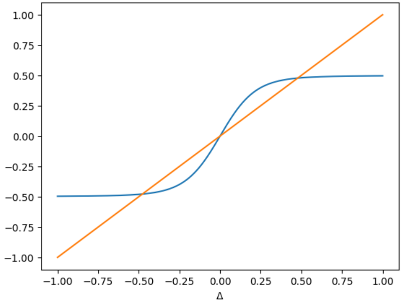

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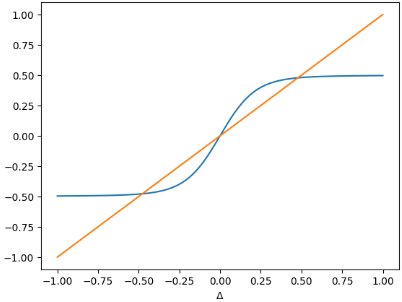

The goal is to find the points of intersection, for which we use fixed point acceleration and the bisection method.

Analysis: Fixed Point Acceleration

The algorithm works on taking the composition of the function with itself repeatedly until it satisfies the self-consistence form;

$$f(f(f(....)))_n = f(f(f(....)))_{n-1} \tag{24}$$

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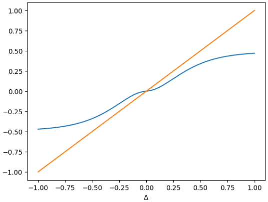
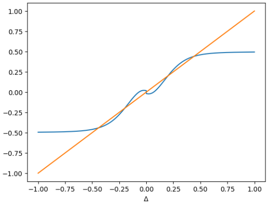
Assuming stability in the fixed point, we find the value of delta.

Analysis: Problems with Fixed Point Acceleration

There are parameters for which, this method fails to find the delta value due to instability.



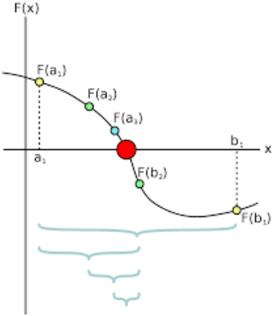
Interestingly, we found that for non zero values of μ, there is another delta value which also satisfies the self consistency equation.



Analysis: Bisection Method

Root-finding method, for;

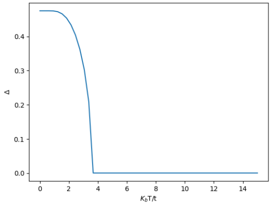
$$f(\Delta) - \Delta = 0 \tag{25}$$



Helps access unstable points, and the extra delta points. The choice goes to the delta value with the least energy, for the ground state.

Δ vs T

Using the above mentioned methods, we plot the variation of delta vs Temperature for varying parameters



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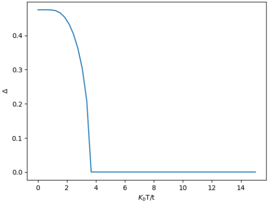

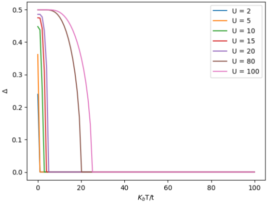

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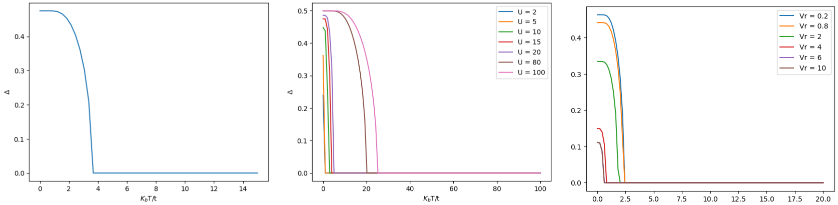


For varying U (Hubbard Parameter) and varying Spin-Orbit Coupling.

Analysis: Energy Optimization

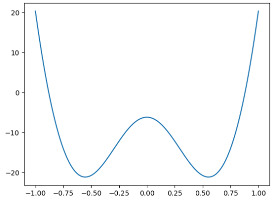
We further tried to verify our self-consistency results to the delta obtained from optimization of energy. We obtained the energy value by taking the expectation of our Hamiltonian (19) for the thermal state which we found to be;

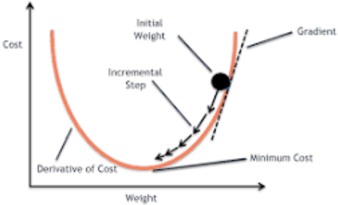
$$
\begin{aligned}
NU\Delta^2 + \sum_k \frac{\epsilon_{k,+}}{2} + \frac{\epsilon_{k,-}}{2} \\
- \frac{E_k^+}{2} \tanh\left[\frac{\beta(E_k^+ - \mu)}{2}\right] - \frac{E_k^-}{2} \tanh\left[\frac{\beta(E_k^- - \mu)}{2}\right] \qquad (26)
\end{aligned}
$$

where, $E_k^{+/-}$, are the final eigenvalues, while $\epsilon_{k,+/-}$ are the the spin-orbit eigenvalues.

Analysis: Gradient Descent

One can see clearly from the graph that it has minimas for varying deltas;





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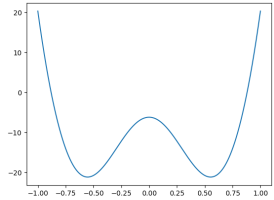
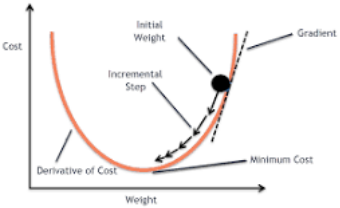
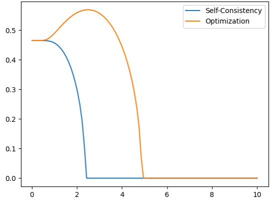




By applying gradient descent we can find the exact delta value for energy minima.

Comparison between Energy Optimization and Self-Consistency

In finding the minima for the function and comparing the delta values with that from the self-consistency equation we got;



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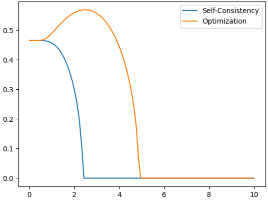
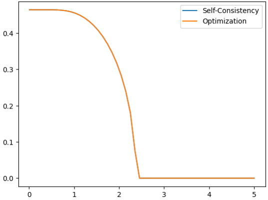


At this point we were suggested to minimize the free energy instead.

Free energy optimization

In doing the free energy optimization we got;



There is a perfect match now. It was understood that, in general one must optimize the free energy;

$$F = U - TS \tag{27}$$

Interestingly, in the graph before we saw the graphs matching initially, which aids the idea that at lower temperatures, one can still work with energy minimization

Section 4

Further directions

Further Directions

- Topological phases and symmetries
- Delve into looking at a 2-D Hamiltonian model to possibly explain superconducting to magnetic order phase transitions
- Observe Hall effects for such models

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*Nat Commun **7**, 13037 (2016)*

Github Link

Thank you!!