A Machine Learning-Enabled Study of Superconductivity

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Application of the XGBoost Algorithm

Rajeev Atla

John P. Stevens High School

July 29, 2020

Outline

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- Introduction
 - Superconductivity
 - XGBoost
- 2 Data
- Methods
- Discussion
- Conclusion
- 6 References
- Acknowledgements

Ginzburg-Landau Theory

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 For a homogenous superconductor, the Ginzburg-Landau equation is

$$\alpha\phi + \beta|\phi|^2\phi = 0$$

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$$\alpha\phi + \beta|\phi|^2\phi = 0$$

• The nontrivial solution for $T < T_c$ is

$$|\phi|^2 = -\frac{\alpha}{\beta} \left(T - T_c \right)$$

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$$\alpha\phi + \beta|\phi|^2\phi = 0$$

• The nontrivial solution for $T < T_c$ is

$$|\phi|^2 = -\frac{\alpha}{\beta} (T - T_c)$$

• The characteristic length scale ξ is called the Ginzburg-Landau coherence length

$$\xi = \sqrt{\frac{\hbar^2}{2m^*|\alpha|}}$$

Types of Superconductors

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• Two types - Type 1 and Type 2

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- Two types Type 1 and Type 2
- Notation

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- Two types Type 1 and Type 2
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 - $H_c(T)$ is critical field as a function of temperature

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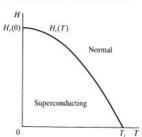


Figure: H - T phase diagram for a Type 1 superconductor [Tinkham]

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 \bullet Ginzburg-Landau parameter $\kappa>\frac{1}{\sqrt{2}}$

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• Ginzburg-Landau parameter $\kappa > \frac{1}{\sqrt{2}}$

• Definition: $\kappa = \frac{\lambda}{\xi} = \frac{e\hbar}{m_{\rm e}c} \sqrt{\frac{\beta}{2\pi}}$

Surface energy is negative

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$$\bullet \ H_{c2} = H_{c1} \kappa \sqrt{2}$$

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• In type 1,
$$H_{c2} = H_{c1}$$

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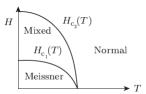


Figure: H - T phase diagram for a Type 2 superconductor [Girvin and Yang 2019]

Type 2 Superconductors: Abrikosov Lattice Vortices

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• For $H_{c1} < H < H_{c2}$ in a Type 2 Superconductor, Abrikosov vortices appear in the material

Type 2 Superconductors: Abrikosov Lattice Vortices

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- For $H_{c1} < H < H_{c2}$ in a Type 2 Superconductor, Abrikosov vortices appear in the material
- These are flux vortices that are quantized, with

$$\Phi = \frac{nhc}{2e}, \quad n \in \mathbb{Z}$$

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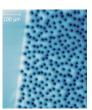


Figure: Abrikosov vortices in YBCO - created by Wells et al. 2015 using scanning SQUID microscopy

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- eXtreme Gradient Boosting
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- Was used to process data from Large Hadron Collider (LHC) [Chen 2015]

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- Ensemble learning [Friedman et al. 2017]

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 - Combination of homogenous weak learners

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 - Combination of homogenous weak learners
 - End result is a weighted sum of weak learners

$$\theta_f = \sum_j w_j \theta_j$$

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XGBoost

- eXtreme Gradient Boosting
- Package for **Python**, C++, Java, R, Julia, and Scala
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- Ensemble learning [Friedman et al. 2017]
 - Combination of homogenous weak learners
 - End result is a weighted sum of weak learners

$$\theta_f = \sum_j w_j \theta_j$$

 w_i are determined by backpropogation via gradient descent

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Taken from UCI (University of California, Irvine)
 Machine Learning Repository

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- Taken from UCI (University of California, Irvine)
 Machine Learning Repository
- 21,263 examples with 81 features

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- Taken from UCI (University of California, Irvine)
 Machine Learning Repository
- 21,263 examples with 81 features
- Model was only trained with 11 features to prevent overfitting

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- Taken from UCI (University of California, Irvine)
 Machine Learning Repository
- 21,263 examples with 81 features
- Model was only trained with 11 features to prevent overfitting



Figure: UCI Machine Learning Repository

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- XGBoost library
 - XGBClassifier class

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• Confusion matrix made using matplotlib library

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Confusion matrix made using matplotlib library

Positive (1) Negative (0) Positive (1) TP FP Negative (0) FN TN

Actual Values

Figure: Example Confusion Matrix

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 Python training files, these slides, the dataset, etc. can be found at https://github.com/ RajeevAtla/Graphene-Research/

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Reference

- Python training files, these slides, the dataset, etc. can be found at https://github.com/ RajeevAtla/Graphene-Research/
- Easiest way to access is using git

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Acknowledgements

I would like to thank Leo Lo and Dr. Serena McCalla for their mentorship through the iResearch Institute.



I would also like to acknowledge my parents for their constant support.