An Analytical Method for Computing the Pair Correlation Functions of Dislocation Loops

Andrew Valentini
Advisor: Prof. Joseph Anderson, Physics and Astronomy Department
Carthage College

Abstract

Dislocations are a type of defect or irregularity in the structure of a material that is otherwise ordered and crystalline. These dislocations either extend across the entirety of a material or self-terminate, forming a loop. Dislocation loops are an important subject of research in solid state physics as well as in materials science because they are the fundamental carriers of deformation in metals. Modeling the distribution of these dislocation loops is crucial to understanding material properties, such as predicting the plastic response of metals. Previous research has developed pair correlation functions for dislocation loops, which describe the relative arrangement of pairs of dislocation lines, using a stochastic geometric approach. In this work, we summarize this geometric approach and propose an alternative method based on Fourier analysis for computing these dislocation loop correlations. We discuss the benefits of this proposed method and consider applications to other linear objects such as cosmological defects.

Defects in Materials and Dislocation Loops

Defects are irregularities in an otherwise ordered material that are typically directly manifest in the structure of a material's lattice structure. The structure of ordered materials always includes some imperfections.

Dislocations are a type of line defect that involve the translation of one part of a material with respect to another.

Any dislocation line that forms a closed curve is called a *dislocation loop*.

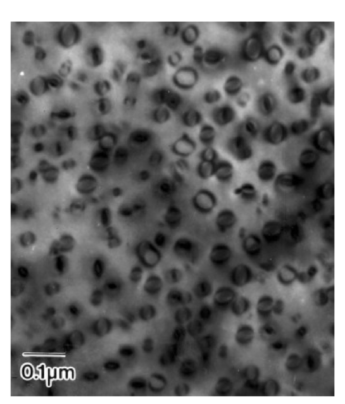

Figure 1. Dislocation loops in a silicon wafer after annealing for 8 hours at 900°C [1].

Pair Correlation Function and Distribution of Dislocation Loops

The pair correlation function $g(r)$ is typically a measure of how likely one is to find something like a particle at a radial distance r away from a given reference point.

This quantity is of interest because allows you to describe properties of interacting objects, such as the average energy of those interactions.

Given a material randomly populated with circular defects, we similarly want a measure for the amount of line length from these circular defects that would be collected inside a radial distance r from a reference point.

We assume that the surface of a material has been randomly populated by circular defects through a Poisson point process.

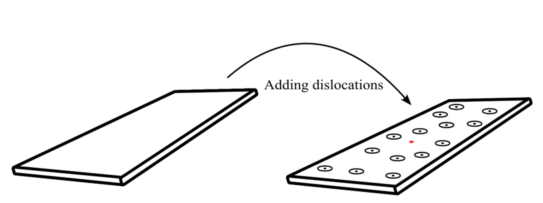

Figure 2. Randomly populating the surface of a material with circular defects. Given a randomly selected reference point on this material (shown in red), how much line length is collected from these loops at a radial distance r away the reference?

Notice that if the material is given a surface density of loops ρ (in units of line length per area) and if one specifies their reference point to *not* land on one of the loops, the amount of line length collected by a radial distance r from this reference will just be given by $g(r) = \rho\pi r^2$.

Stochastic Geometric Approach

You must also consider what happens when you specify your reference to originate *on* one of the defect loops to develop a full correlation function. This is more subtle than before; now there is a nonuniform distribution of line length. This was first considered on the following geometric grounds in [2]:

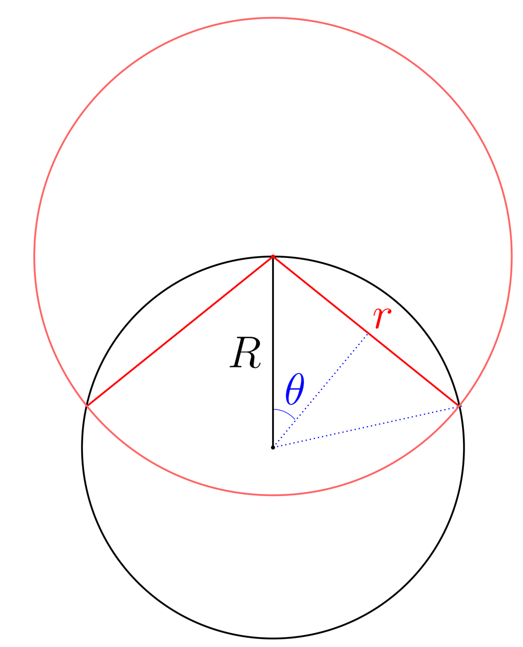

Figure 3. The setup of the problem. The black circle is the defect of radius R and the red circle is the radial distance r from your origin location which has been specified to exist *on* the loop.

The radius r forms a chord of the loops when $r > R$ so half the total opening angle θ is given by

$$\theta = \arcsin\left(\frac{r}{2R}\right). \tag{1}$$

The total line length $L(r)$ inside our radial distance r is therefore

$$L(r) = \rho\pi r^2 + 4R\arcsin\left(\frac{r}{2R}\right) \tag{2}$$

since our angle θ only captures half of the total line length on *one side* of the loop.

The line length *at* a radial distance r is given by the density of line in the small differential area produced when r is changed, meaning the line density at a distance r from your origin will be:

$$\rho(r|\text{disl. at } 0) = \rho + \frac{1}{2\pi r}\frac{\partial L}{\partial r} = \frac{1}{\pi r\sqrt{1-\left(\frac{r}{2R}\right)^2}}. \tag{3}$$

The resulting correlation function is then

$$g(r) = \frac{1}{\rho\pi r\sqrt{1-\left(\frac{r}{2R}\right)^2}}. \tag{4}$$

Analytic Approach

The Fourier transform of a loop with density $\rho(\boldsymbol{r})$ is given by:

$$\mathscr{F}_1\{\varrho(\boldsymbol{r})\} \equiv \hat{\varrho}(\boldsymbol{k}) = \frac{1}{\sqrt{2\pi}}\int_{\mathbb{R}^3} e^{-i\boldsymbol{k}\cdot\boldsymbol{r}}\varrho(\boldsymbol{r})d^3\boldsymbol{r} \tag{5}$$

which can be expressed as

$$\hat{\varrho}(\boldsymbol{k}) = \frac{1}{\sqrt{2\pi}}R\int_0^{2\pi} e^{-i\boldsymbol{k}\cdot\boldsymbol{r}_l(\theta)}d\theta \tag{6}$$

since the loop's density is the Dirac delta function:

$$\varrho(\boldsymbol{r}) = \int_{\mathcal{L}} \delta(\boldsymbol{r} - \boldsymbol{r}_l)d\boldsymbol{l} \tag{7}$$

(it only has a nonzero density along the radial coordinate where the loop is defined, $\boldsymbol{r}_l$). This turns out to be the definition of the zeroth order Bessel function when $\boldsymbol{k}$ is written in its polar form so we have

$$\hat{\varrho}(\boldsymbol{k}) = \sqrt{2\pi}RJ_0(|\boldsymbol{k}|R). \tag{8}$$

Analytic Approach Continued

To arrive at a pair correlation from this approach, we must convolve the expression in Eq. (8), which is a way of combining two separate signals which allows you to look at how they are correlated.

By the convolution theorem, the pair density is therefore

$$\begin{aligned}(\varrho * \varrho)(\boldsymbol{r}) &= \mathscr{F}_2^{-1}\{\hat{\varrho}(\boldsymbol{k})\hat{\varrho}^*(\boldsymbol{k})\} \\ &= 2\pi R^2\mathscr{F}_2^{-1}\{J_0^2(|\boldsymbol{k}|R)\}.\end{aligned} \tag{9}$$

Results

After laboring at Eq. (9), we found that

$$\frac{1}{2\pi r}\frac{\partial}{\partial \phi}\left(2\pi R^2\mathscr{F}_2^{-1}\{J_0^2(|\boldsymbol{k}|R)\}\right) = \frac{1}{\pi r\sqrt{1-\left(\frac{r}{2R}\right)^2}} \tag{10}$$

where ϕ is a variable from one of the Bessel functions of Eq. (9).

This tells us that the full pair correlation function will be given by

$$g(r) = \frac{1}{\rho\pi r\sqrt{1-\left(\frac{r}{2R}\right)^2}} \tag{11}$$

which exactly matches Eq. (4)!

We have shown that our proposed analytic approach to computing the pair correlation function of dislocation loops yields the same result as the stochastic geometric approach originally developed by [2].

Cosmological Defects and Future Work

Dislocation loops and *defect loops* have been intentionally used interchangeably in this poster. This problem was initially posed in the context of dislocation loops but this method can be applied to find the correlation of any type of circular line object.

The analytic method we have developed provides the benefit of being able to generalize easier to more complicated pair correlation functions.

To pursue personal interests, we plan to apply this method to study cosmic strings, which are hypothetical topological defects in the universe which are theorized to have resulted from a vacuum phase transitions in the early universe.

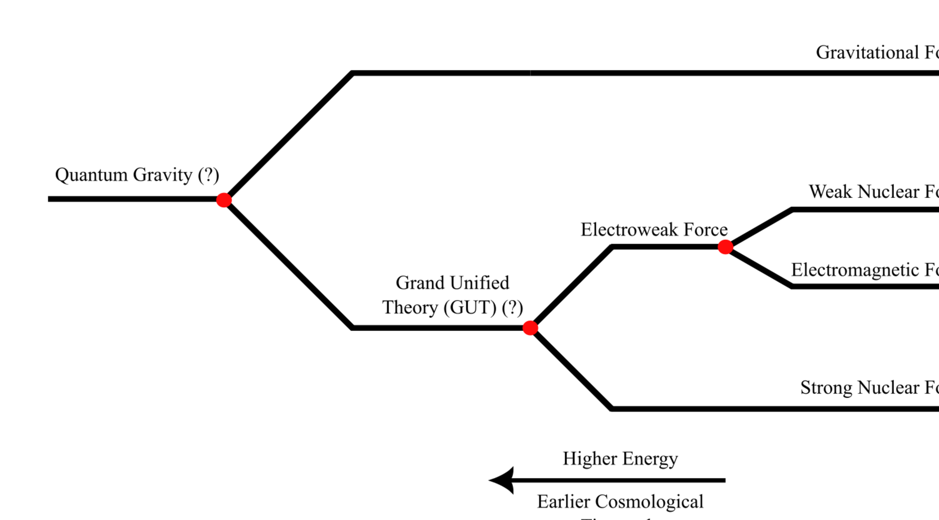

Figure 4. A chronological diagram of the sort of hypothesized symmetry breaking in the early universe which may have given rise to cosmic strings and other topological defects

Taking the Fourier transform of a pair correlation function results in a power spectrum, which is a distribution of energy across frequencies. We therefore plan to develop a model for the background gravitational radiation from these cosmic strings.

References

[1] L. Robertson and K. Jones, "Silicon: Defect evolution," pp. 8533–8543, 2001.

[2] H. Stoyan and D. Stoyan, "Simple stochastic models for the analysis of dislocation distributions," *physica status*

avalentini@carthage.edu