

Correcting Phonon and Quasiparticle Dynamics in Geant4 Simulation of Kinetic Inductance Detectors

Ruth Berkun

Abstract

Kinetic Inductance Detectors (KIDs) can be used to detect low-mass dark matter candidates. When dark matter interacts with KIDs, it creates a pulse of phonons and quasiparticles, the latter of which can be used to characterize the energy of the dark matter. However, the physics behind phonon propagation and interaction with quasiparticles is not well understood. To gain more insight into these interactions, we modify a previous Geant4 (GEometry ANd Tracking) simulation created by a previous lab member (Erik Lindeman) and compare it to experimental data of a lab wafer of KIDs. Upon seeing that there are key differences in quasiparticle pulse shapes between simulated and experimental data, we try to see if the implemented phonon physics could be causing these discrepancies. The modified physics in E. Lindeman's simulations were found to create a disproportionate amount of gap-energy phonons (phonons whose energy is twice the bandgap energy of the KIDs or feedline), as well as to cause KIDs closer to the initial energy deposit to absorb many more phonons than far away KIDs. More work needs to be done to understand how these phonon physics features are affecting the quasiparticle pulses. Understanding such interplay of phonon and quasiparticle physics can help aid the development of more sensitive detectors.

Introduction

Astronomical and cosmological observations suggest that the universe contains a missing-matter component, called “dark matter” (DM) [1]. Theoretical developments have posited the existence of low-mass DM candidates, with masses less than that of a proton of 1 GeV. When these DM candidates interact with regular matter, they may only deposit very small amounts of energy within a target, on the order of a few eV [2]. Such interactions require sensitive, high resolution radiation detectors to observe. One such device is kinetic inductance detectors (KIDs) [4].

The composition of KIDs allows them to detect small energy deposits. KIDs are composed of thin, superconducting aluminum films layered on a silicon crystal. In the aluminum, electrons travel together in pairs (Cooper pairs) instead of repelling, leading to near-zero resistance and hence superconductivity [5]. When energy is deposited within the Si crystal from an external particle interaction, lattice vibrations known as phonons are produced and propagate through the crystal [6]. These phonons can be absorbed by the thin-film aluminum, breaking their constituent Cooper pairs and creating quasiparticles (collective excitations) [5]. The change in Cooper pair density and increase in quasiparticle density is measured as a change in inductance in the circuitry of KIDs [6].

To better understand and aid the development of KIDs, the physics of phonon propagation and subsequent absorption by a superconductor will need to be simulated. The Golwala group has built several working

detectors that consist of arrays of KIDs, which have detected energy deposits (from controlled radioactive sources) under 1 MeV [4]. However, the exact physics of these detectors, such as how phonons are generated and decay over time, and how phonons determine quasiparticle density, is not completely understood. A previous student in the Gowala group, E. Lindeman, carried out a Geant4 (GEometry ANd Tracking) simulation based on a detector (an array of KIDs) developed by the Golwala lab in 2012 [4]; however, the results of the simulation, while broadly matching observed pulse shapes, showed key differences from experimental data collected (as seen in Figure 1) [7].

In this project, we aim to refine, validate, and expand the existing KID simulation to match the previous experimental data, but for an 80-KID device [8] as opposed to the 2012 prototype [4]. Lindeman had a separate version of his simulation using the 80-KID device's geometry, and preliminary analysis of that simulation suggests that the simulated and experimental pulses differ in several ways (Figure 1). The simulated pulses take longer to decay than their experimental counterparts and reach their peaks later. Plus, the time of pulse peak and decay rate as a function of KID distance from initial energy deposit differs for the simulated vs experimental data. Due to these disparities in the existing KID simulation, we need to make changes to it to match experimental data.

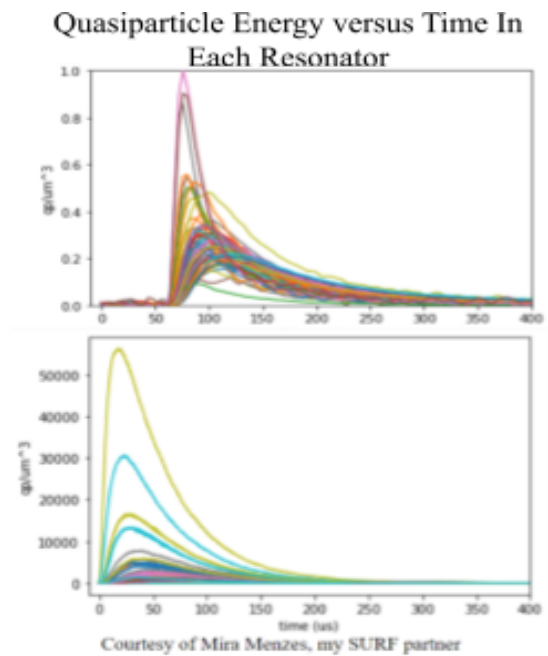


Figure 1: Energy response of the 20 KID 2012 design [4] with experimental data (top) and simulation output (bottom). Though broad features have been captured, the relative pulse heights and decay times across sensors are inconsistent between Monte Carlo output and measurements.

To find the root of these differences, we examine the phonon and quasiparticle physics separately. We will study whether changes from library defaults have caused the phonon distributions to deviate from their expected shapes. Correcting issues with the phonon physics first will prevent confusion from which quasiparticle pulse discrepancies arise from faulty phonon versus quasiparticle physics.

Materials and Methods

Software dependencies

All simulations are being run on the Caltech HPC (High Performance Cluster); however, this is simply for ease of access because the HPC already has the required software packages installed. If running the simulations of the KIDs remotely, it is recommended to install PuTTY (Popular SSH and Telnet Client, for accessing and running remote files) and Xming (for viewing simulation output images). The Visual Studio Code Remote - SSH extension is also very useful for editing remote files in a typical IDE

(Interactive Development Environment) if one does not want to do everything via Vim and the command line.

To run the simulations of the KIDs locally, one needs a Linux or MacOS operating system or emulator. Python 3.8.5, Cmake version 3.3 or up, C++ 11, and gcc (C++ compiler, version 10.3.0) must be installed. Only then can the Geant4 package (10.6.3p3) be installed, as well as the supporting library G4CMP (“A low energy condensed matter physics package for Geant4”).

Building on Previous Work

The lab has already done some work on improving quasiparticle physics in the films. Because G4CMP is an evolving platform, it hasn’t implemented comprehensive quasiparticle physics in its KaplanQP class. Its quasiparticles release phonons to decay into lower energy quasiparticles, but quasiparticles never recombine to create phonons.

A student, Erik Lindeman, implemented a version of KaplanQP that did perform recombination in his own simulation. It takes an amount of energy called the gap energy of a material to create quasiparticles. In Lindeman’s modified KaplanQP simulation, within a certain range of the gap energy, quasiparticles downconvert to the gap energy. There they can recombine with other gap energy quasiparticles to create gap energy phonons.

We suspect that E. Lindeman’s version of KaplanQP has introduced changes to the phonon physics that are unphysical. In Figure 2, we compare the distribution of phonons in Lindeman’s modified KaplanQP simulation to a simulation of a CALDER detector, from a paper on Geant4 simulation we call the “CALDER paper” [4]. While KIDs are not arranged the same way on the CALDER detector as our detectors, the detector compositions are similar, making their phonon distributions somewhat comparable. Compared to the CALDER phonons absorbed in KIDs, the modified Kaplan simulation is absorbing phonons of lower energy overall, less than 1.5 THz. Additionally, there are unphysical spikes near the gap energies of the KIDs and feedline.

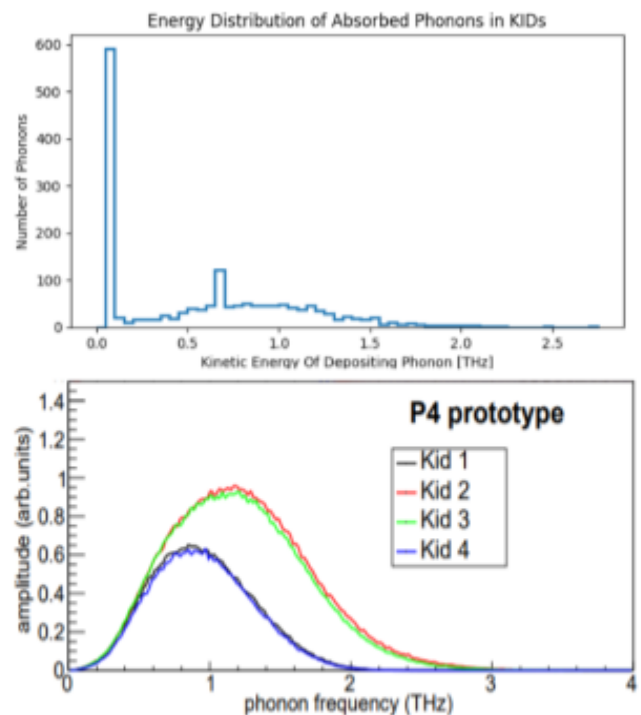


Figure 2: Kinetic energy of phonons that are absorbed into the all the KIDs of each detector after a 3.2 eV energy deposit. Top: simulated data (80-KID detector). Bottom: CALDER simulation [8] (4-KID detector). Notice that the phonons in the top graph are lower frequency than those of the bottom, and have spikes the bottom distributions do not.

My work will involve investigating whether these changes to quasiparticle recombination affect phonon distributions created by this modified KaplanQP simulation. First, we create a simplified simulation, without any of the fancy modified KaplanQP stuff, with just one KID on it. This isolates effects on phonons caused by multiple KIDs, and also lets us more directly compare to the simple geometries of the CALDER paper. If our phonon distributions match those of the one-KID prototype in the CALDER paper, we can move onto the second step, which is importing the geometry of our lab's 80-KID detector that we simulated in the modified KaplanQP simulation. Comparing our simple, unmodified KaplanQP simulation to the modified KaplanQP simulation, we will see the effects of Kaplan modifications on phonon distributions. The workflow of investigating the effects of modified KaplanQP is illustrated in Figure 3.

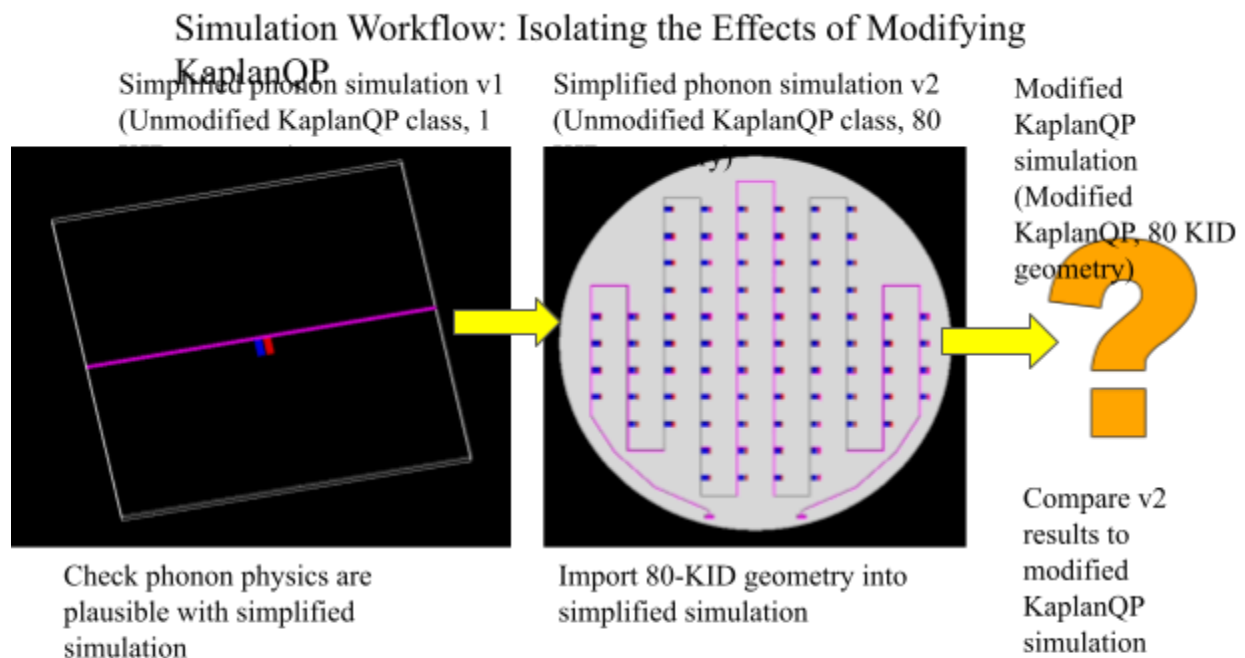


Figure 3: Workflow showing the different simulation versions that are made to determine where strange phonon distribution features are coming from. The images show the geometry of the 1 KID detector (left) and 80 KID detector (right). In both images, the feedline is pink, the capacitors are blue, and the inductors are red.

Results and Discussion

Simplified simulation v1: 1-KID geometry

While creating the simplified 1 KID simulation, I discovered there were multiple absorption parameters that could determine what phonons got absorbed into the KIDs:

- **pAbs:** A “naive” absorption parameter. If pAbs is set to n%, it randomly selects n% of all phonons to get absorbed into the superconducting film of the KIDs. Otherwise, the phonon is reflected. In both cases, KaplanQP is not involved and thus quasiparticles are not created.

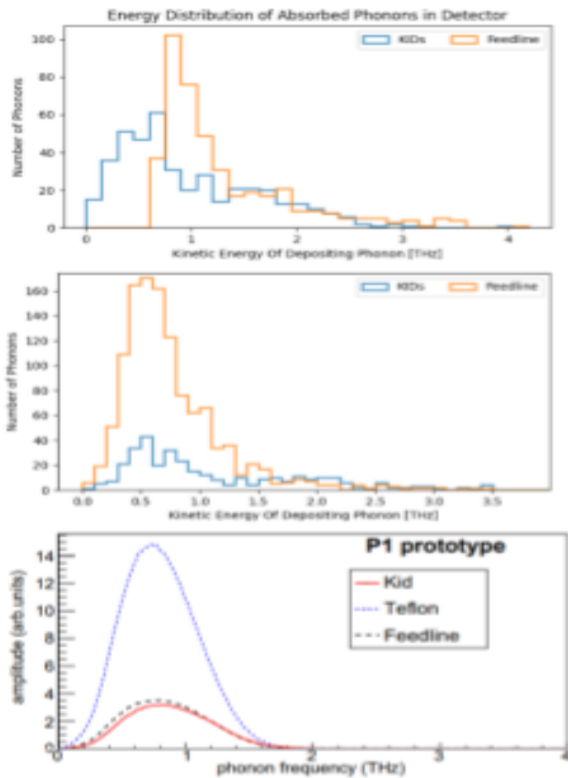


Figure 4: Histogram distribution of energies of phonons that are absorbed in single KID (1-KID geometry).

Top: simplified simulation v1, filmAbsorption = 0.1.

Middle: simplified simulation v1, pAbs = 0.1

Bottom: CALDER paper, 1 KID prototype (P1). Due to the distribution shape similarity to the middle figure, it is suspected that pAbs and not filmAbsorption was set for this CALDER simulation.

- **filmAbsorption:** Like pAbs, if filmAbsorption is set to $n\%$, then $n\%$ of all phonons will enter the film. However, unlike pAbs, not all these phonons will automatically get absorbed. filmAbsorption calls upon KaplanQP, meaning that the phonons that enter the film can be absorbed and create quasiparticles, or get reflected back into the silicon immediately without being absorbed.

In figure 4, the effect of setting pAbs versus filmAbsorption in the simplified simulation is compared. When setting pAbs, the distribution of absorbed phonons matches the CALDER paper pretty well, with the exception of a small tail of higher energy phonons, probably from the initial energy deposit downconverting. By contrast, when setting filmAbsorption, the shape is less symmetric and more skewed right than the CALDER distribution.

From this it seems likely that pAbs was used to create the distribution in the CALDER paper instead of filmAbsorption.

Despite setting pAbs creating more similar looking distributions to the CALDER paper, we decide to stick with filmAbsorption instead. When setting pAbs, there is no interface to KaplanQP at all, and thus absorbed phonons don't create quasiparticles. Setting filmAbsorption, however, does trigger quasiparticle dynamics. While it causes the distribution to be less even than those in the CALDER paper, lots of new phonons are created from quasiparticles in the film, escape the film, and can get absorbed by the KIDs again. Because we believe quasiparticle dynamics are important for our KID response, we use filmAbsorption for the rest of this project, in both the modified KaplanQP and simplified simulations. We will no longer compare to the CALDER paper, which focuses on phonon physics only and seems to use pAbs instead.

Even though we aren't trying to exactly match the CALDER paper distributions anymore, we see that we have met our original goals for correcting unwanted gap energy spikes in the phonon distribution, and we

are also finally absorbing > 1.5 THz phonons. Thus, these phonon physics seem well-enough behaved for us to move onto our second step, simulating with our lab's 80 KID geometry.

Simplified simulation v2: 80-KID geometry

Even after adding 80 KIDs to the simplified simulation, the gap energy spikes did not return (Figure 5). Thus, we can confirm that those spikes were caused by the modified Kaplan physics creating a lot of gap energy phonons from quasiparticles recombination inside the film. We know that these gap energy phonons often escape the film and end up in the silicon, so it makes sense that more gap energy phonons in the silicon creates a disproportionate chance for gap energy phonons to get absorbed in the KIDs.

We also see that both simulations are absorbing phonons mostly below 2 THz, which is less energy than the phonons in the 1 KID sim. Also, in the simplified simulation, the peak of phonons absorbed is closer to 0.25 THz than 0.5 THz like the peak in the 1 KID sim. Thus we can infer that more KIDs on a detector causes lower energy phonons to dominate. This may be because when a greater percentage of the surface area of a detector is covered with KIDs, even low-energy phonons have a higher chance to get absorbed. And because low energy phonons dominate in the film over time (all phonons must eventually decay to lower energy phonons), they are absorbed disproportionately more.

Lastly, KIDs were grouped by distance from initial energy deposit to see how that affected the average phonons absorbed in each group (Figure 6). The modified KaplanQP simulation had the closer KIDs

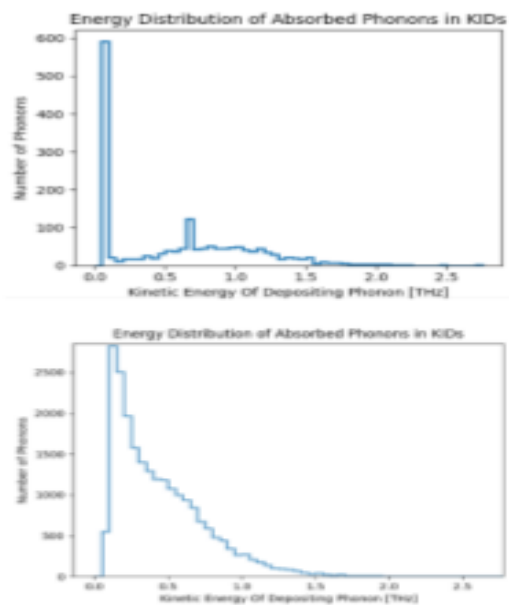


Figure 5: For 80 KID geometry, comparison of absorbed phonon energy distribution over all KIDs. Top: modified KaplanQP simulation. Bottom: simplified simulation v2.

The simplified simulation no longer has the same strange spikes as the modified Kaplan simulation, but is notable skewed right and lacks > 1.5 THz phonons, features it did not have as a 1 KID simulation.

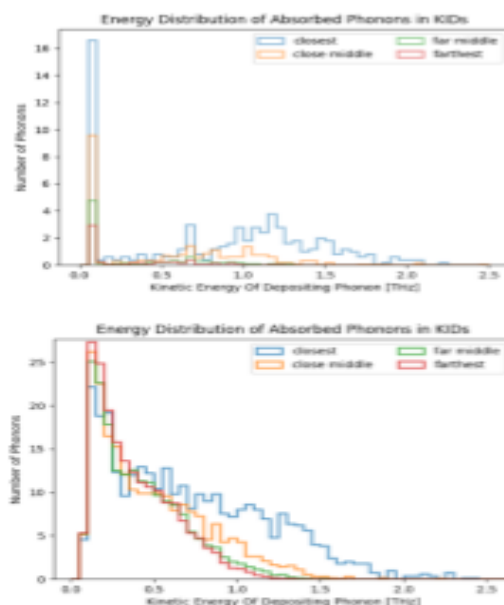


Figure 6: For 80 KID geometry, comparison of absorbed phonon energy distribution over KID close and far from initial energy deposit. Top: modified KaplanQP simulation. Bottom: simplified simulation v2.

KIDs are grouped based on their distance from the initial energy deposit. Because there are more KIDs at a far radius from the energy than near, the groups are not the same size. Thus the Y axis displays the average number of phonons for any single KID in each group.

The modified KaplanQP version has a notably more uneven distribution

absorbing a lot more phonons on average than those far from the energy deposit. By contrast, in the simplified 80-KID simulation, KIDs near and far from the energy depository absorbed more similar distributions of phonons, the only exception being that the closest KIDs absorbed more phonons above 1 THz.

While it makes sense that the farther from your initial energy deposit you go, the less chance a phonon will travel out that far, we still need to compare each KID's phonon distribution to its quasiparticle pulse to truly understand the effect of distance. The modified Kaplan simulation shows some KIDs having quasiparticle pulses that are way too low, hinting that the modified Kaplan simulations's far KID phonons might be too few, but this requires further investigation.

Conclusion

In summary, we worked on isolating the effects of modifying KaplanQP's quasiparticle physics on distributions of phonons absorbed by the KIDs. We learned that due to how the modified kaplanQP recombines quasiparticles, there are a disproportionate number of gap-energy phonons that exist in the detector and get absorbed. We saw that modified kaplanQP caused KIDs closer to the initial energy deposit to absorb many more phonons than far away KIDs. And in both modified and simple KaplanQP simulations, we saw that adding more KIDs caused more low-energy phonons to be absorbed.

In the future, we want to relate our new understanding of these features in the modified KaplanQP phonon distributions to the quasiparticle distributions. We now know a non-physical amount of gap-energy phonons are being absorbed in KIDs, but is this causing strange features in our distributions as well? And are differences in phonon energies absorbed by near and far KIDs causing unwanted quasiparticle distributions as well?

Overall, we have a better understanding of phonon distributions, but need to relate them to the quasiparticle pulses so we can experimentally validate them.

References

- [1] Arkani-Hamed, N., Finkbeiner, D. P., Slatyer, T. R., & Weiner, N. (2009). A theory of dark matter. *Physical Review D*, 79(1). <https://doi.org/10.1103/physrevd.79.015014>
- [2] Kouvaris, C., & Pradler, J. (2017). Probing sub-gev dark matter with conventional detectors. *Physical Review Letters*, 118(3). <https://doi.org/10.1103/physrevlett.118.031803>
- [3] Echternach, P. M., Pepper, B. J., Reck, T., & Bradford, C. M. (2017). Single photon detection of 1.5 thz radiation with the quantum capacitance detector. *Nature Astronomy*, 2(1), 90–97. <https://doi.org/10.1038/s41550-017-0294-y>

- [4] Moore, D. C., Golwala, S. R., Bumble, B., Cornell, B., Day, P. K., LeDuc, H. G., & Zmuidzinas, J. (2012). Position and energy-resolved particle detection using phonon-mediated microwave kinetic inductance detectors. *Applied Physics Letters*, 100(23), 232601. <https://doi.org/10.1063/1.4726279>
- [5] *What are Cooper Pairs & how are they responsible for superconductivity?* Science ABC. (2022, March 23). Retrieved February 19, 2023, from <https://www.scienceabc.com/pure-sciences/what-are-cooper-pairs-how-are-they-responsible-for-superconductivity.html>
- [6] Shaw, M. D., Bueno, J., Day, P., Bradford, C. M., & Echtermach, P. M. (2009, March 13). *The quantum capacitance detector: A concept for a pair-breaking radiation detector based on the single Cooper-Pair Box*. arXiv.org. Retrieved February 19, 2023, from <https://arxiv.org/abs/0902.4194>
- [7] Lindeman, E (2020), *DMKID Phonon Monte Carlo Simulation* [PowerPoint slides]. Internal Documentation
- [8] Golwala, Sunil, et al. A Massive, Position-Resolving, High-Energy-Resolution Detector for Non-Accelerator Cosmic and Intensity Frontier Particle Physics. No. DOE-CALTECH-0013881. California Institute of Technology (CalTech), Pasadena, CA (United States), 2022.
- [9] Martinez, M. *et al.* Measurements and simulations of athermal phonon transmission from silicon absorbers to aluminum sensors. *Physical Review Applied* **11**, (2019).