Electron Transportation in Geant4 Condensed Matter Physics Simulation for Use in Searches for Dark Matter

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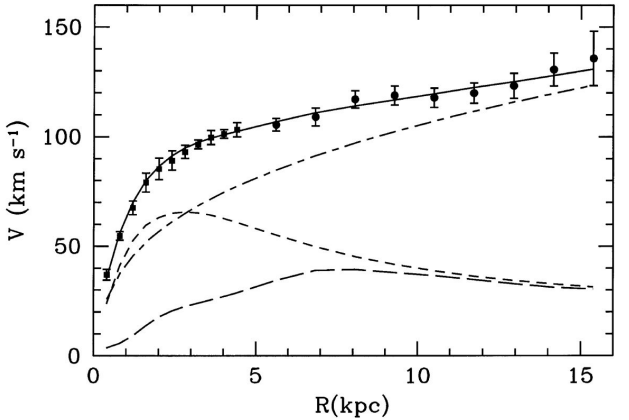
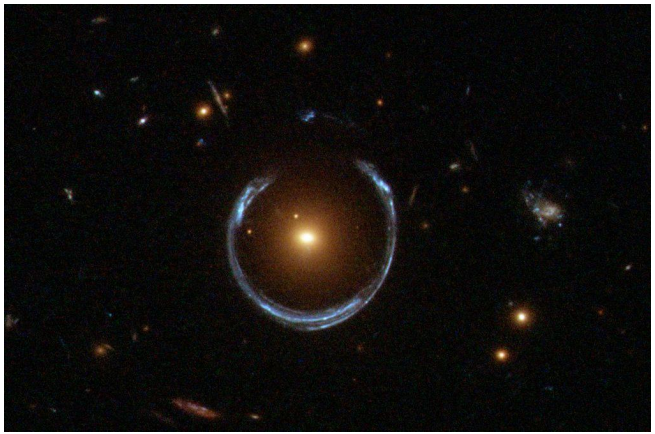
Outline

- Introduction and Motivation
  - The Dark Matter and Super Cryogenic Dark Matter Search Experiment (SuperCDMS)
  - SuperCDMS Detector Simulations
  - Charge Propagation in Semiconductor Crystals
- Dominant Effects in the Electron Transportation in a Semiconductor Crystal
  - Energy-Momentum Relationship
  - Electric Field
  - Scattering Effects
- Simulating the Dominant Effects with a Toy Simulation
  - Trajectories
  - Arrival Positions at the Top Surface
- Summary and Next-Steps
- Overview of the Geant4 Condensed Matter Physics (G4CMP) Addon
- Conclusion

The Mystery of Dark Matter

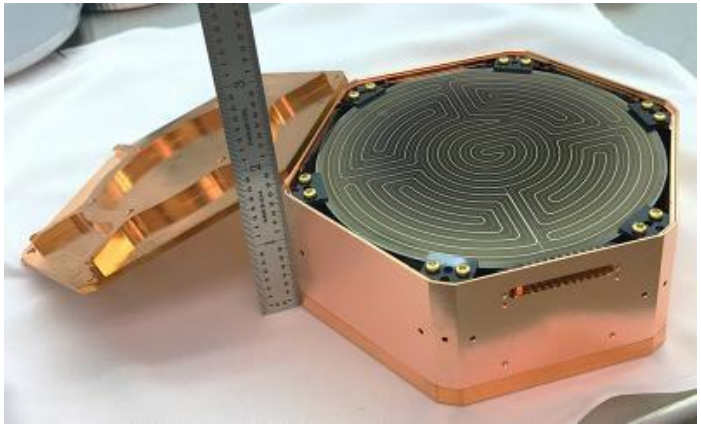
- Observed gravitational effects in the universe cannot be fully explained by visible matter alone
- Dark matter is proposed to account for this "missing" mass, influencing galaxy formation and cosmic structure
    - Stars at galaxy edges move faster than predicted if only visible matter is considered (top figure)
    - Gravitational lensing patterns (Einstein rings) around distant galaxies are different from the observed size from the visible matter alone
- Simplest solutions: Weakly Interacting Massive Particles (WIMPS) are hypothetical particles that barely interact with normal matter, making them nearly invisible





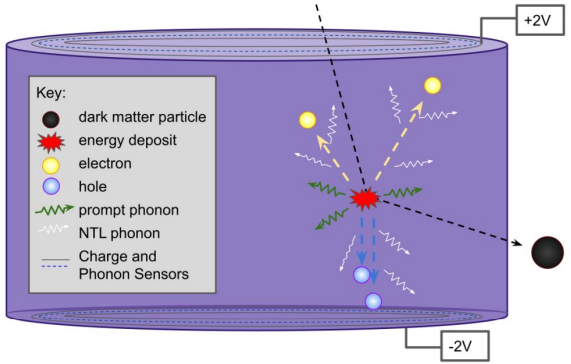
Super Cryogenic Dark Matter Search Experiment (SuperCDMS)

- The Super Cryogenic Dark Matter Search Experiment (SuperCDMS) is designed to directly detect particle dark matter in the form of WIMPs or other models
- The Super Cryogenic Dark Matter Search Experiment (SuperCDMS) is based on detectors made from silicon or germanium in the millikelvin temperatures to measure small energy particle interactions



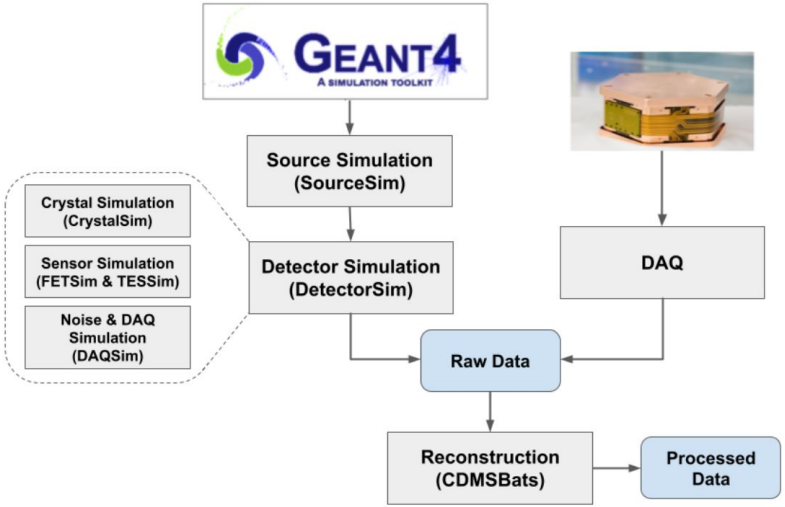
Super Cryogenic Dark Matter Search Experiment (SuperCDMS)

- When either standard model particle or dark matter particles hit a detector, they deposit their energy and excite electrons from the lattice to form an electron-hole pair and emit phonons
- Electrons travel through the detector, scatter, and emit phonons, until they hit the top of the detector where they are measured by sensors
- High quality measurements of the charges and phonons allows us to separate between dark matter and SM backgrounds



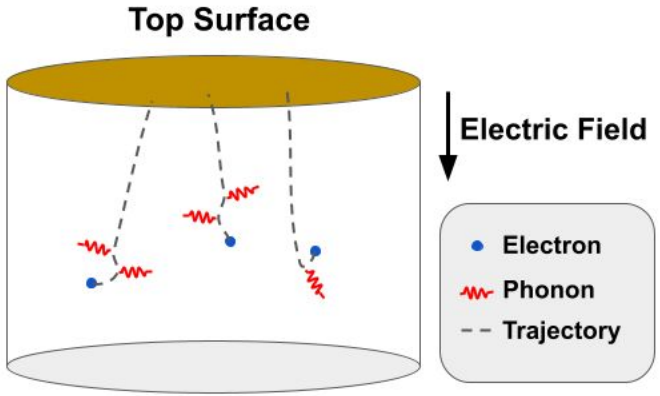
SuperCDMS Detector Simulations

- A high quality simulation allows us to better understand how to differentiate between dark matter and SM particle interactions
- The simulation needs to model the correct charge and phonon physics in a semiconductor detector (G4CMP)
- In this thesis, we will focus on the charge transportation physics simulation and how it produces phonons



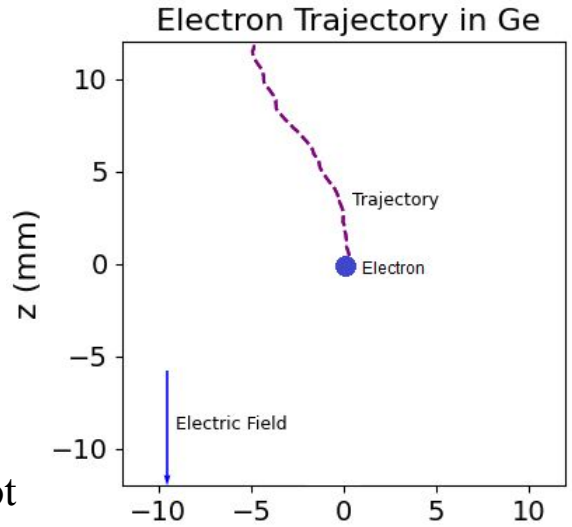
Charge Propagation in Semiconductor Crystals

- In a detector, what we see are the patterns that electrons and holes form on the top and bottom surface sensors after traveling to the surface
  - In this discussion we are going to focus on the electrons
- Our goal is to understand and predict these patterns and model the motion of an electron and its phonon production in a semiconductor for use in the SuperCDMS detector simulation
- For the sake of time, we are going to skip the derivation and simply show the results with more details in the backup slides
- We are going to start from the simplest case then introduce the dominant effects one at a time



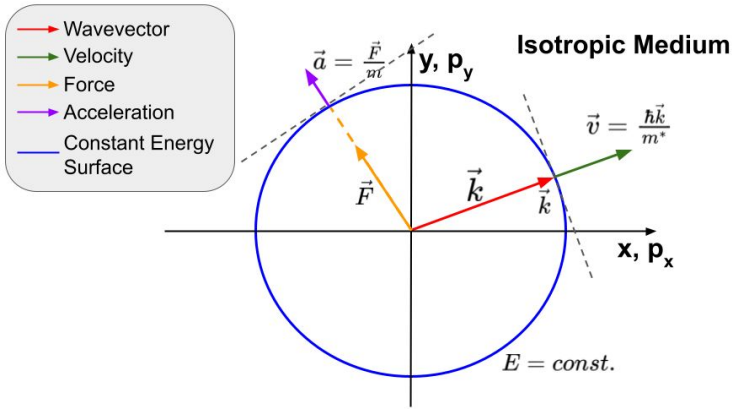
Charge Propagation in Semiconductor Crystals

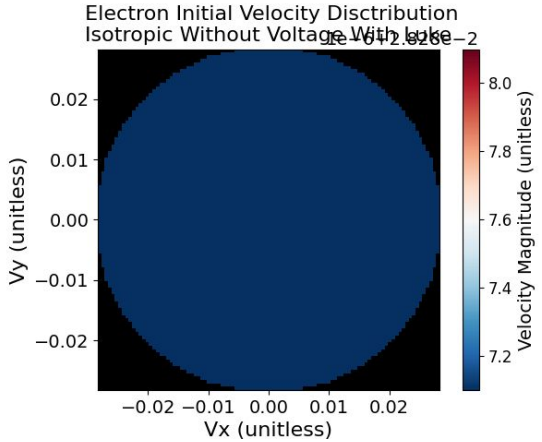
- Motion of an electron through a crystal lattice has a number of complex effects which need to be taken into account to explain the full trajectory
- The most important is that the lattice causes a periodic potential in the electron's Schrödinger equation, which leads to effects that are purely Quantum Mechanical in nature and make the motion non-intuitive
- We will cover three general effects:
  - Effect 1: There are certain directions in which electrons move more slowly; these are referred to as "valleys"
  - Effect 2: The direction and magnitude of any acceleration is not only a function of an external force, but is also a function of the crystal orientation
  - Effect 3: Electrons can scatter within the crystal either from the lattice or other particles



Charge Propagation in an Isotropic Medium (Simplest Case)

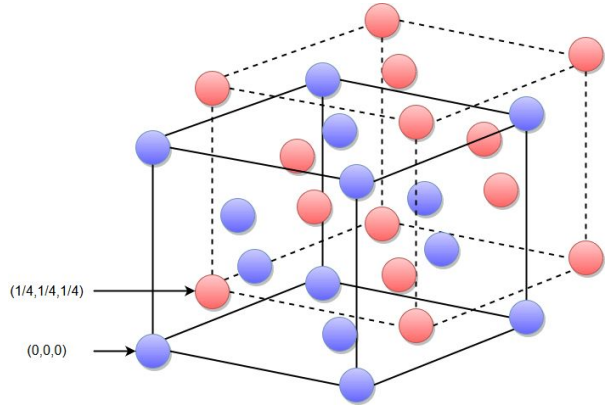
- Starting with the case we are used to (and there are no surprises), the figure shows a two-dimensional image of the relationship between the kinetic energy of a particle in a medium and its wavevector
  - Example cases: vacuum or an isotropic medium which is a material that has uniform properties in all directions
- Note that the velocity and acceleration are in the same direction as the wavevector and force respectively
  - Can think of the blue circle in the top figure as a constant energy "surface"
- The bottom plot shows that the velocity distribution is the same for any initial velocity direction





Effect 1: Energy is Different in Different Directions

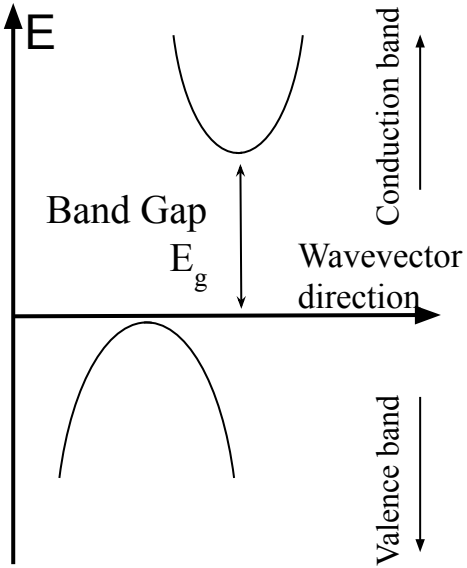
- Semiconductor crystals have an anisotropic lattice structure which gives different directions in space different properties
- The periodic band structure leads to a periodic potential in the Schrodinger equation
- Bloch's theorem implies that the wavefunctions of the charges in a periodic lattice can be expressed as periodic functions in wavevector[1] space
- The periodicity in both physical space and wavevector space allows the formation of continuous, periodic energy bands with extrema



1. Wavevector Definition

Effect 1: Energy is Different in Different Directions

- We refer to the directions of the lowest energy level as **Valleys**[1]
  - Six valleys in Silicon
  - Eight valleys in Germanium
- For a low-temperature crystal (like those in SuperCDMS Detectors), the band gaps are 1.166eV for silicon and 0.7437eV for Germanium[2]



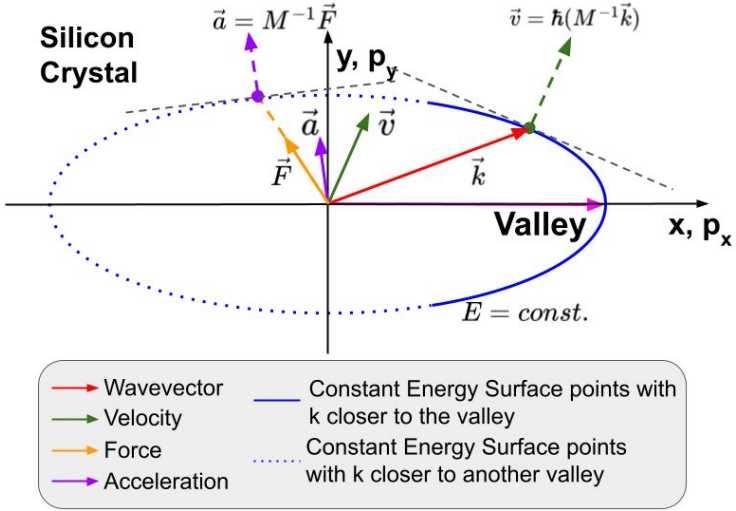
1. Notable Directions in the Conduction Band
2. Low Temperature Band Gaps

Moving to Motion in the Crystal Without Derivation

- The solutions also show that the trajectories are well-modeled by classical motion in a vacuum but where different directions have different "mass"

Free Electron	$E_{kin} = \frac{1}{2}\frac{p^2}{m_0} = \frac{1}{2}m_0v^2$	$v = \frac{p}{m_0} = \frac{\hbar k}{m_0}$	$a = \frac{F}{m_0}$
Electron in Crystal	$E_{kin} = \frac{1}{2} < p\|M^{-1}\|p >= \frac{1}{2} < v\|M\|v >$	$v = M^{-1}p = M^{-1}\hbar k$	$a = M^{-1}F$

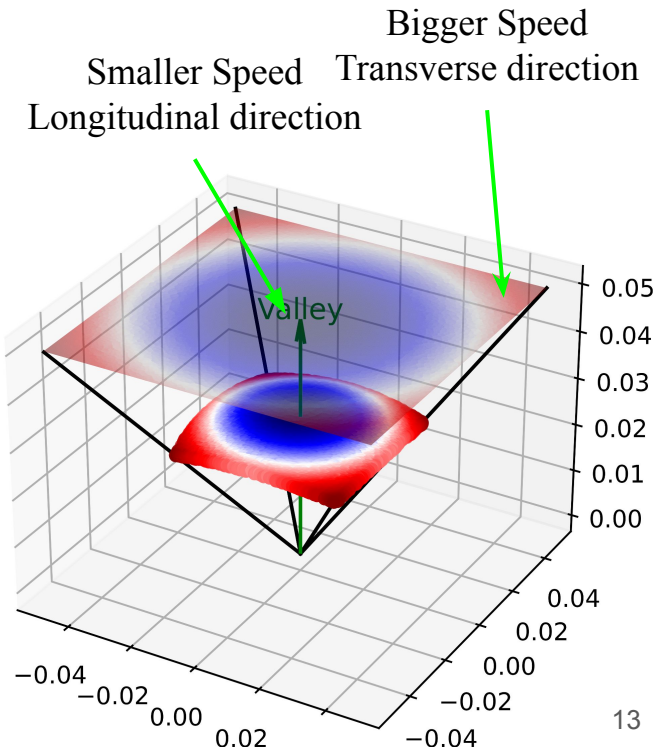
- The mass term in the equations becomes a 3x3 matrix which essentially includes the information about the crystal: Refer to this as **<u>Mass Tensor</u>, M**
- In an anisotropic medium, the velocity and acceleration directions are governed by the mass tensor and are not necessarily in the same direction as the wavevector and force



Mass Tensor and Momentum Magnitude for a Single Valley

- We can consider all motion local, and move to a frame where the x-axis is along the valley direction
  - We refer to the valley direction as longitudinal, and the other two as being transverse
  - In this frame the mass tensor becomes diagonalized and well described by two different masses. Previous experiments have measured these effective masses
- We call the $p=\hbar k=Mv$ the **quasi-momentum**[1] and $P=m_0 v$ the **transport momentum** or just **momentum**
- As the longitudinal mass is bigger than the transverse mass, same energy electrons with a speed (or momentum) direction closer to the valley have a smaller speed (momentum) magnitude

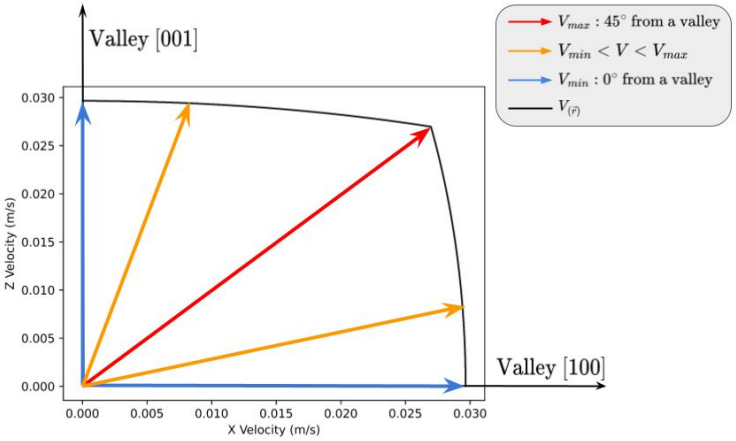
$$M = \begin{bmatrix} m_l & 0 & 0 \\ 0 & m_t & 0 \\ 0 & 0 & m_t \end{bmatrix}$$

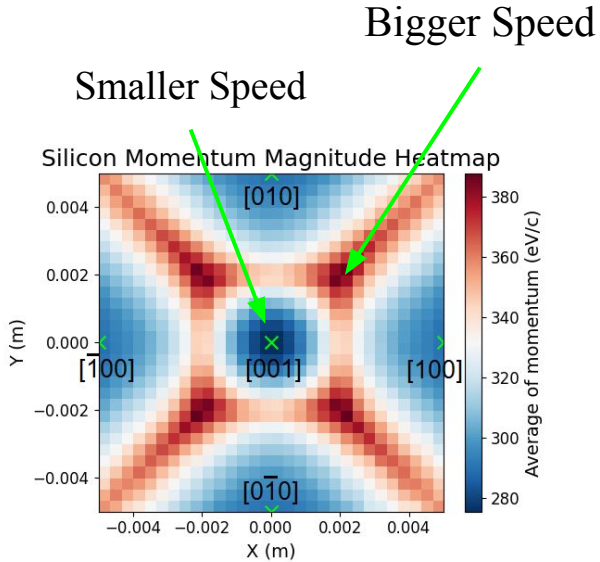


1. Also known as crystal momentum

Moving to More Than One Valley

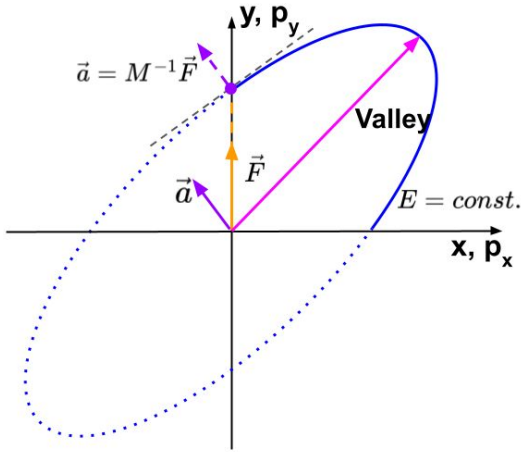
- The top figure shows the electron speed as a function of it's direction between two valleys
  - Note the maximum and minimum as a function of direction relative to the valley
- The bottom figure again shows the momentum distribution at the top surface when we include all Silicon valleys

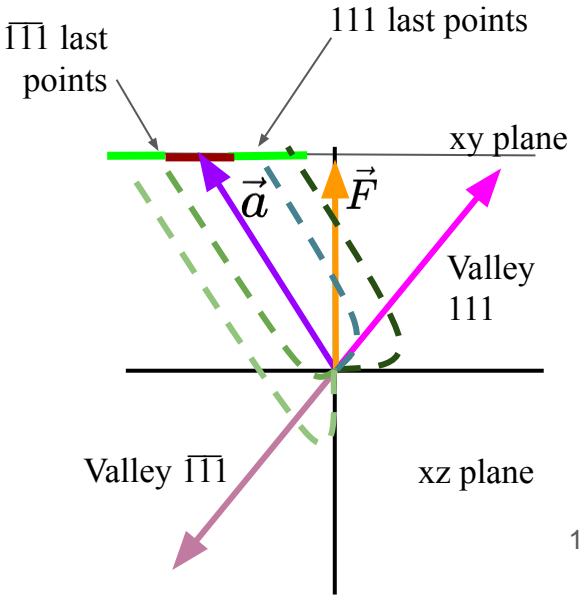




Effect 2: Charge Transport Under an Electric Field Without Scattering Effects

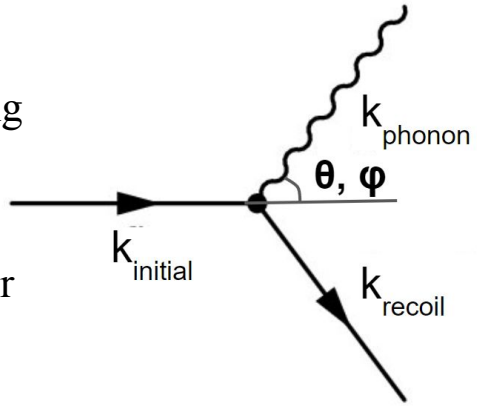
- When there is a force in the semiconductor crystal the acceleration and force are not necessarily in the same direction
- The acceleration and trajectories from the origin are shown as solid and dashed lines in the bottom plot, for a Germanium crystal where we have chosen to have the force in a direction different than a valley (like in the CDMS experiment)
- For valleys on the same axis but in opposite directions, the electrons in both valleys will have the same acceleration and will end up in a similar location on the top surface





Effect 3: Intravalley (Luke) Scattering in a Semiconductor Crystal

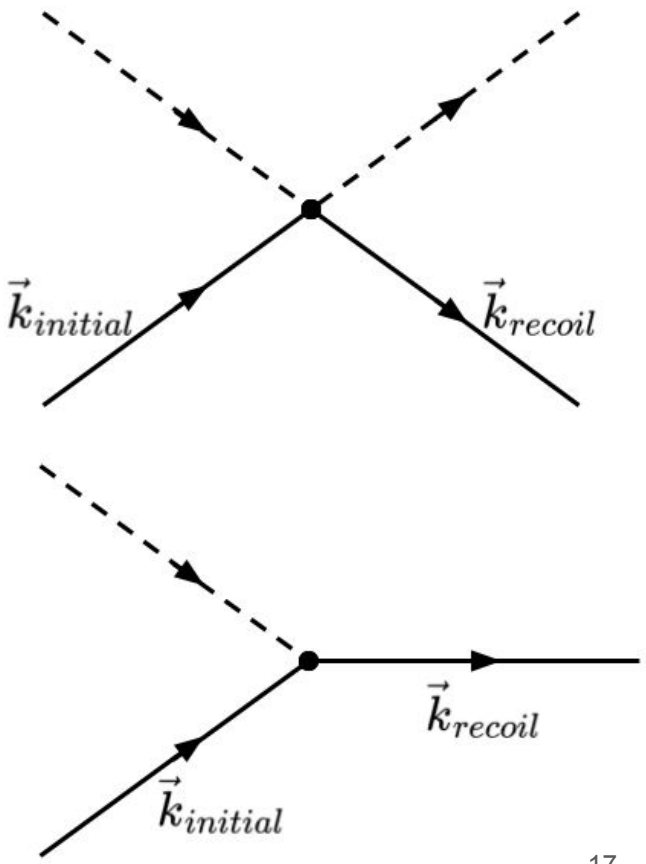
- The electrons can also have interactions within the crystal as they move
- The figure shows a charged particle entering from the left, interacting with an atom in the lattice, and causing vibrations in the crystal (emitting a Neganov-Luke phonon)
    - For low-energy electrons, the scattered electron will typically remain in the same valley. For this reason, we will sometimes refer to it as **intravalley scattering**
    - Other times, we will refer to this as **Luke Scattering** because of the Luke-phonon emitted



- Under an electric field, the electron will get accelerated and gain energy making it more likely for the electron to scatter, emit a Luke phonon, and slow down again
    - This causes the electron to have an effective average speed while creating a lot of Luke phonons which is a central component the CDMS energy measurement
    - The overall direction of the motion is dominated by the acceleration direction
    - The Luke phonons will mostly make a cone around the net electron direction

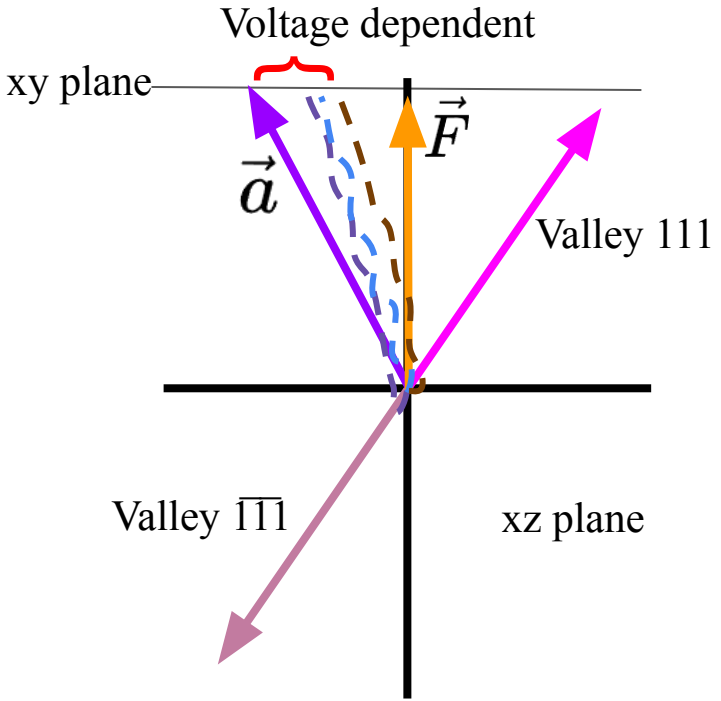
Other Interactions: Intervalley Scattering in a Semiconductor Crystal

- While this won't be important for this presentation, we note two other types of interactions that can impact the trajectory: the top figure shows a charged particle interacting with a second particle and scattering
- The bottom figure shows a charged particle interacting with a phonon and absorbing its energy
- For low energy electrons the particles they encounter are also likely to be of low energy, so changing valleys means switching to one of the same allowed valleys of the same type
- We call these types of scattering Intervalley scattering



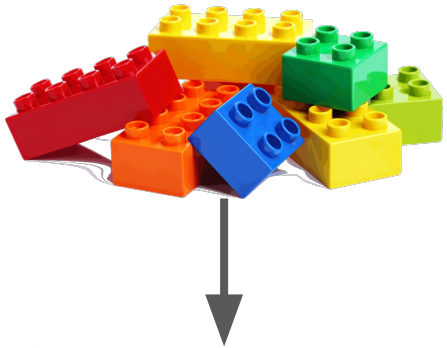
Combining effects: Charge Transport Under an Electric Field With Luke Scattering

- The figure shows the electron trajectories in Ge with both an electric field and including intravalley scattering
- Ultimately, with a voltage, the trajectories will be in-between the acceleration direction and the valley direction
  - The scattering always pulls them towards the valley (bias in the scattering direction)
  - The voltage always pulls them towards the acceleration direction
- The top surface arrival positions will depend on the voltage since the electrons always stay low energy and never switch valleys



Overview and Goals of a Toy Simulation With Only The Dominant Effects

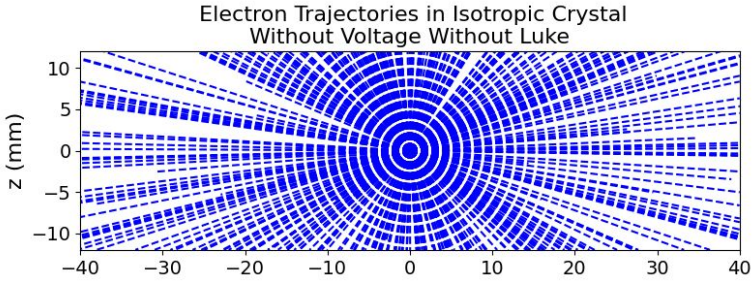
- The full thesis goal is to have a full Geant4 modeling of electrons, holes and phonons
- Our intermediate goal is to ensure that we understand the dominant effects (which helps with development and detector/analysis design)
- In the next slides we present the results of a toy simulation that will be used for comparisons with the full simulation and, eventually, real data (beyond the scope of the thesis)
- We will follow the same order of adding effects, and highlight the differences between the different crystal structures
- In all cases we have simulated a crystal of 80mm x 80mm x 24mm, all with a monochromatic energy and emanating from the center at x=y=z=0

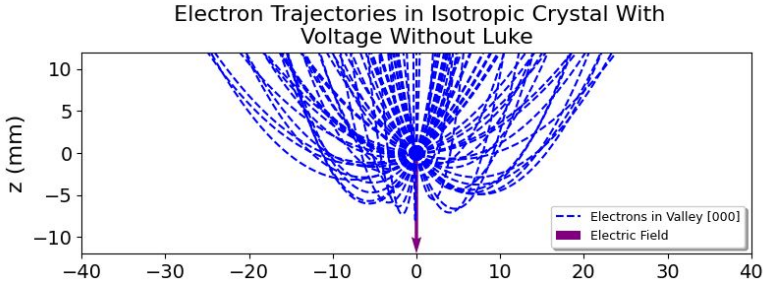


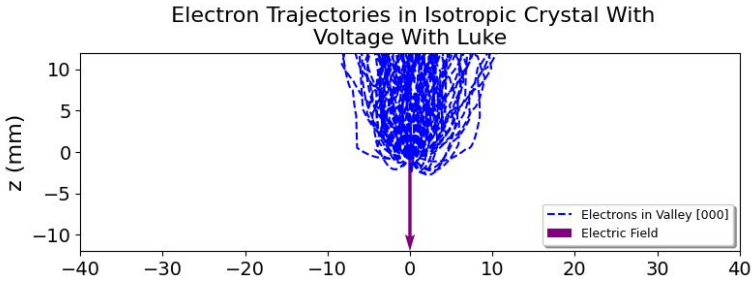
Electron Trajectory in an Isotropic Crystal for All Three Effects

Here we show three versions of the trajectories, shown from the side (xz plane), where the voltage will be pointing downwards and we consider the top surface (z=12 mm)

- The top plot shows the trajectories without voltage or scattering
  - Electrons move in a straight line
- The middle plot shows the trajectories when we add voltage but without scattering
  - Electrons gain acceleration in the same direction as the external force
- The bottom plot shows the trajectories with Luke scattering added
  - Electrons quickly lose energy and their movement is dominated by the acceleration

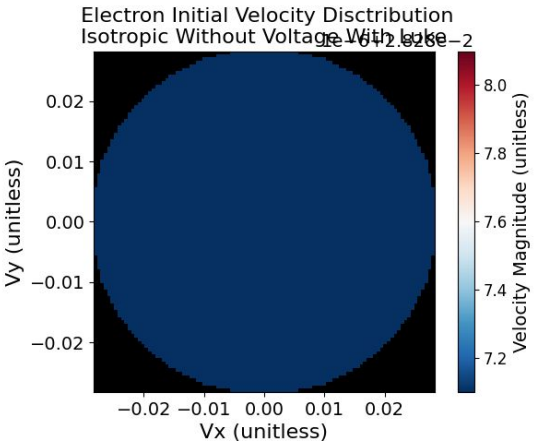


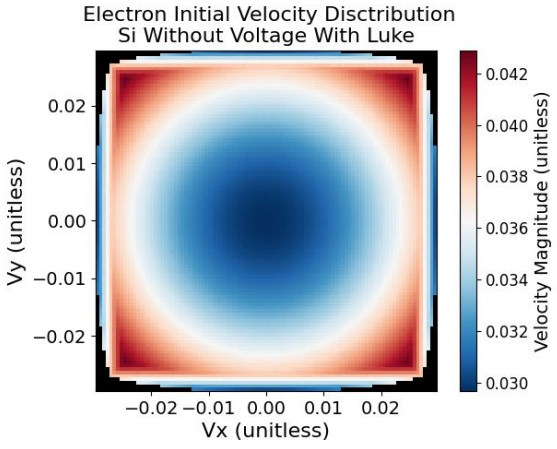


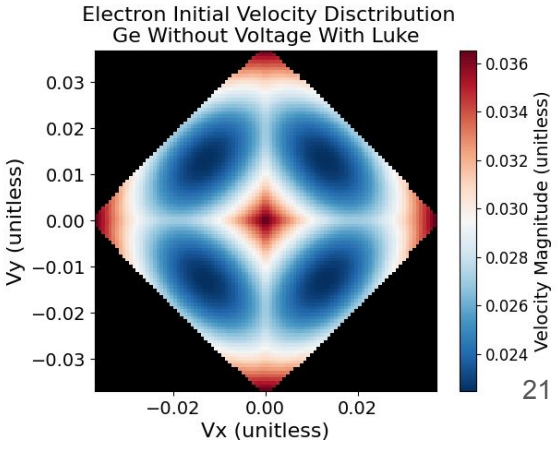


Effect 1: Comparing the Speed Distributions Between Crystal Types

- Moving to the different crystal types, and focusing on just the speed when there is no voltage, we see differences in the speed due to lattice effects
- The figures are not circular (2D projection of a sphere) as the velocity magnitude in the xy plane is also a function the angle with the valleys, which is why there are no colors on the corners (black areas)
- Note that the velocity magnitude is less for the velocities that have less angle with the valleys
    - The isotropic crystal (left plot) has no valleys, so all electrons have the same velocity
    - The Silicon crystal (middle plot) has 6 valleys aligned with the x, y, z axes
    - The Germanium crystal (right plot) has 8 valleys aligned with the (±1,±1,±1) directions

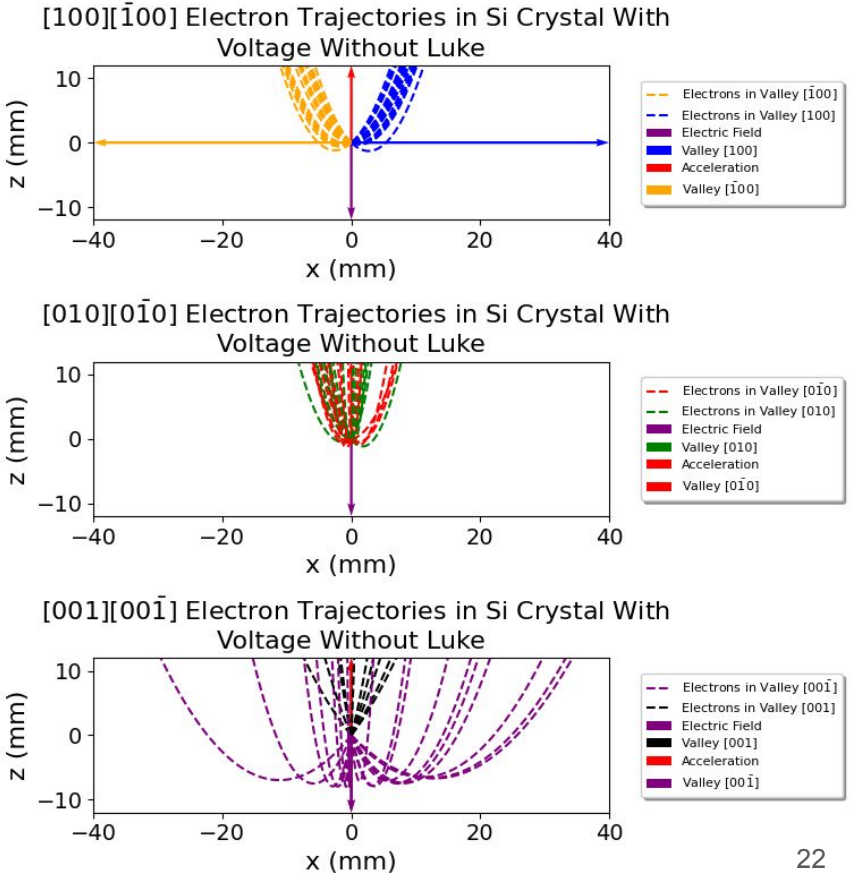






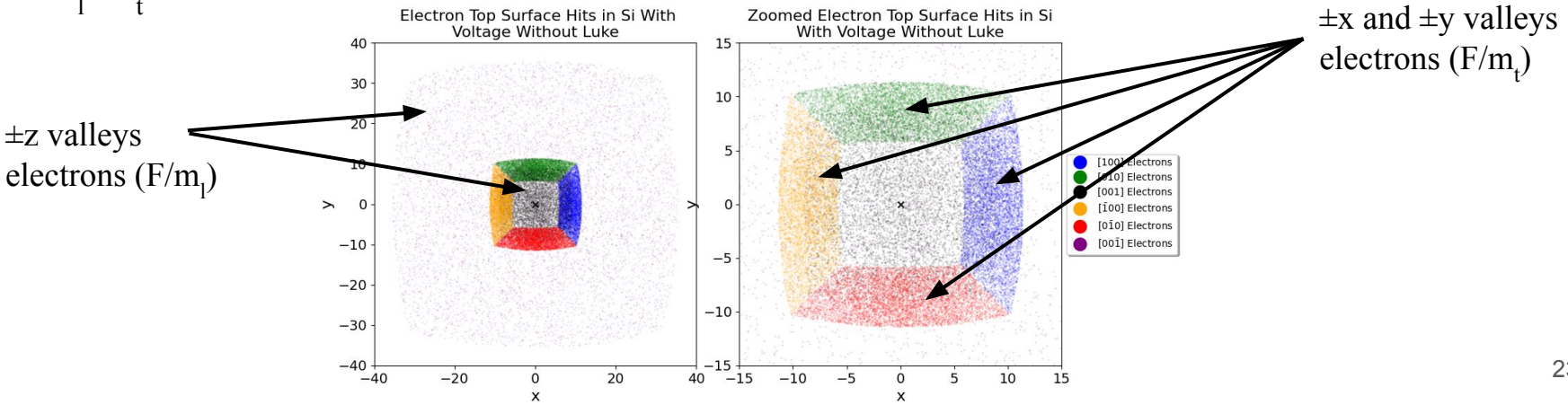
Effect 2: Trajectories in Silicon for Each of the Different Valleys Under an Electric Field Without Scattering Effects

- Starting with the silicon case and adding voltage, we separate the trajectories for pairs of valleys
  - Note that these figures are the same as the middle figure for the isotropic case, but in a silicon crystal
- Note that the acceleration for the z axis valleys (third figure) looks smaller than the x and y axes valleys (first and second figures)
- The second plot is basically looking at the first plot from the side



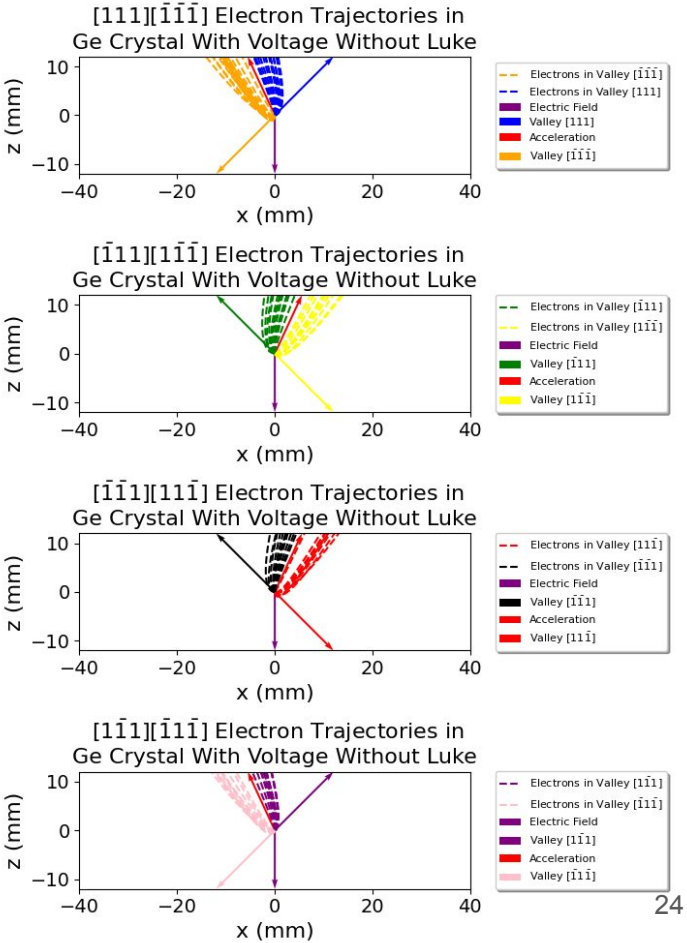
Effect 2: Arrival Positions at the Top Surface in Silicon for Each of the Different Valleys Under an Electric Field Without Scattering Effects

- Next we combine the results from the six valleys, but consider the arrival position at the top surface
- The bottom left plot shows the electrons top surface arrival positions for the same setup (right plot is zoomed in)
- The acceleration direction is the same as the external force as the force is in the same direction or perpendicular to each valley ($a=M^{-1}F$)
- The acceleration magnitude is smaller for the ±z valley (F/m_l) than ±x and ±y valleys (F/m_t), as $m_l>m_t$



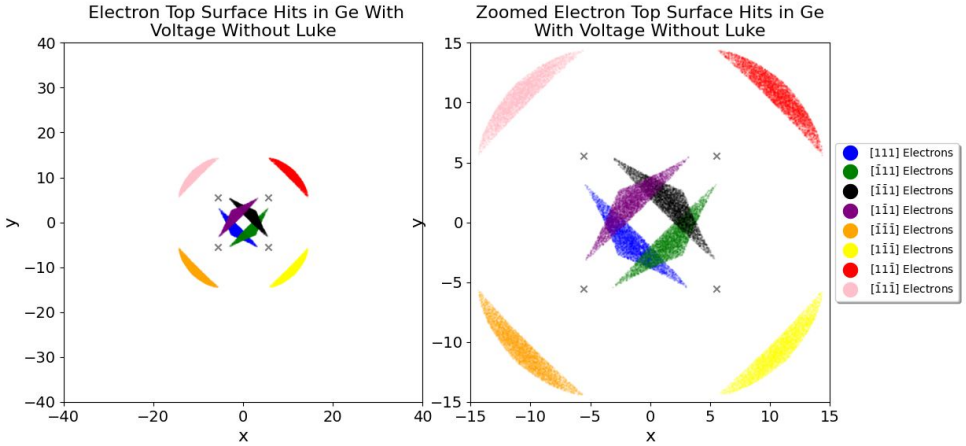
Effect 2: Trajectories in Germanium for Each of the Different Valleys Under an Electric Field Without Scattering Effects

- Again we show the electron trajectories with a voltage, but with pairs of valleys in a Ge crystal aligned with the (±1,±1,±1) directions
- Note that for all 8 valleys none of the acceleration directions are the same as the external force
- As the angle of the valleys with the external case are all the same, the acceleration magnitudes are all the same



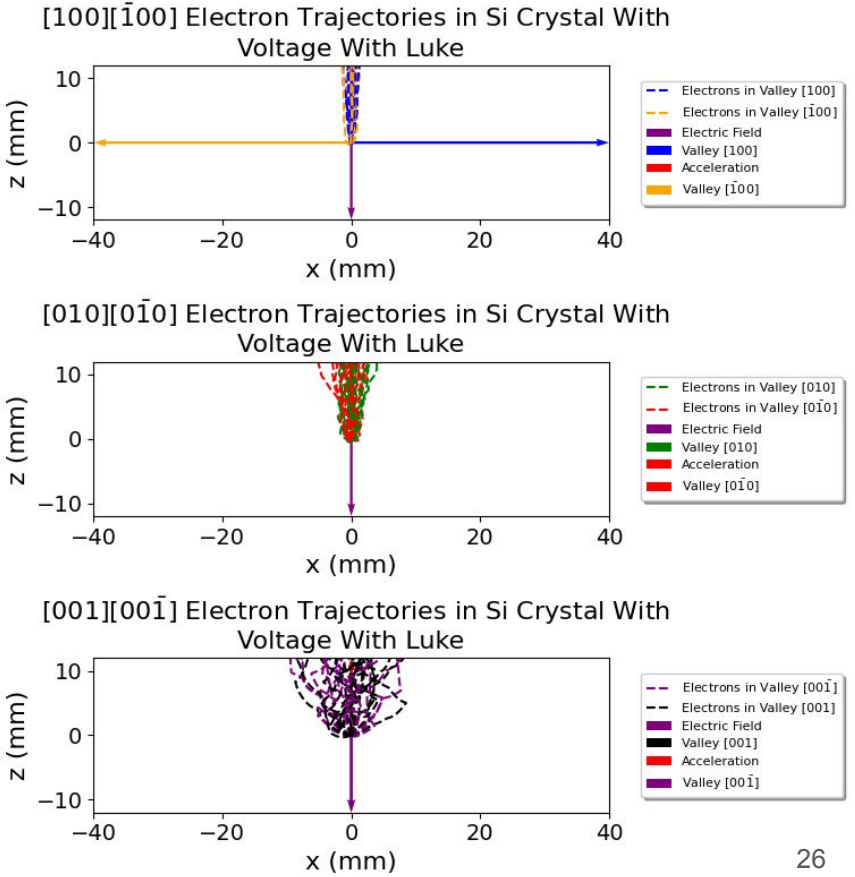
Effect 2: Arrival Positions at the Top Surface in Germanium for Each of the Different Valleys Under an Electric Field Without Scattering Effects

- Again switching to the arrival positions on the top, we see that the Ge case is less intuitive
- The same energy electrons are divided into 8 groups based on their initial momentum direction (8 octants)
- In the absence of the valleys each octant should make a quadrant in the top surface
- But with valleys, the initial momentum magnitude for the same energy electrons is a function of angle with the valleys, which the electrons in the same octants will have different initial momentum magnitude, resulting into the shapes that you see below



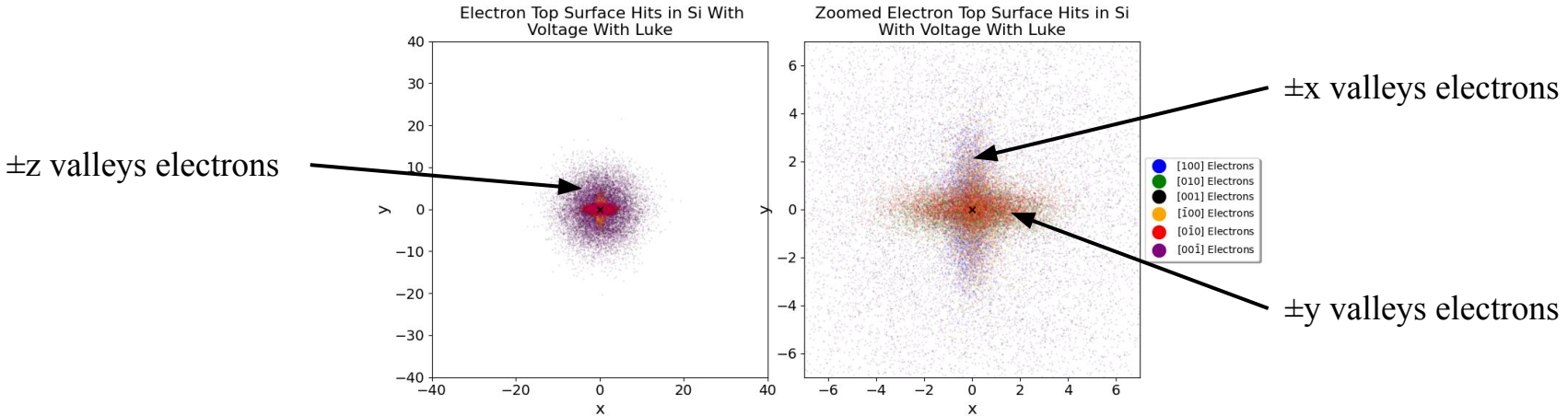
Combining effects: Trajectories in Silicon for Each of the Different Valleys Under an Electric Field With Intravalley Scattering

- Next, we again show the electron trajectories in a silicon crystal, but this time with intravalley (Luke) scattering
- As expected, electrons quickly lose their initial energy and their movement will be dominated by the voltage and scattering
- Comparing the first and the second plots you can notice that the electrons with a higher angle with their valley will have higher initial momentum, which means they initially move further perpendicular to the valley



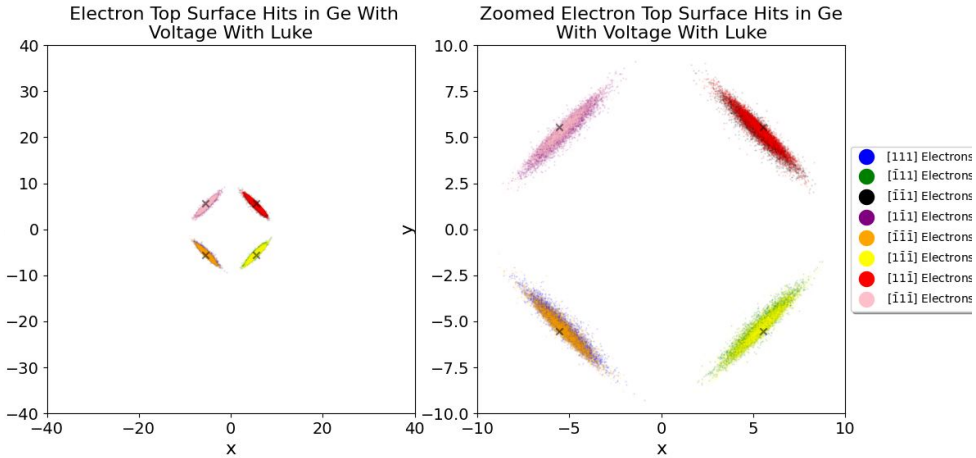
Combining effects: Arrival Positions at the Top Surface in Silicon for Each of the Different Valleys Under an Electric Field With Scattering Effects

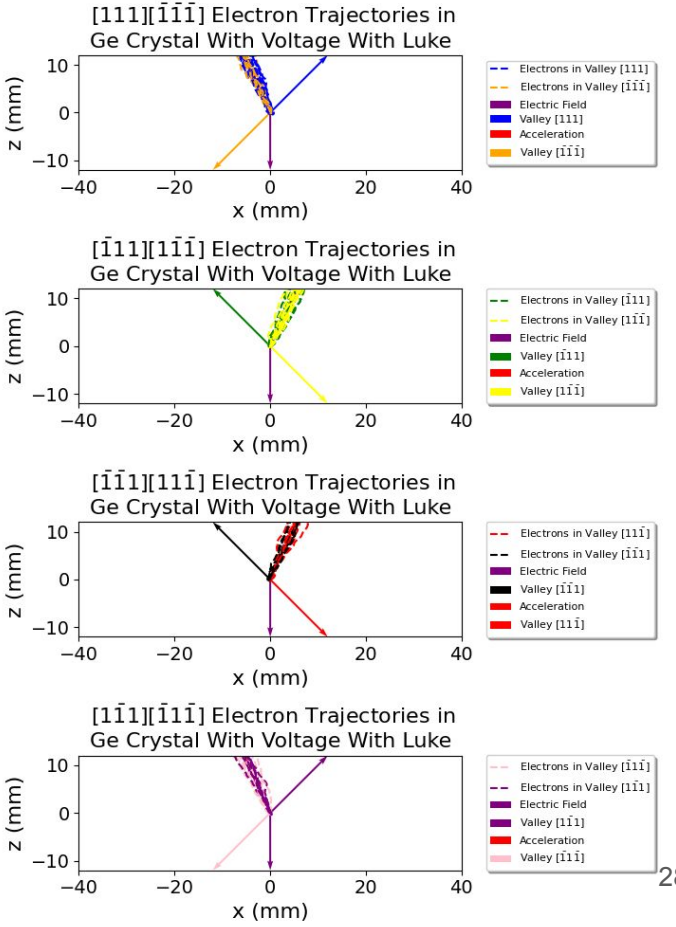
- Next, looking at the arrival positions on the top, we see a different shape than the no-scattering case for silicon
- Note that the arrival positions are much more focused at the center
- The ±x and ±y valleys electrons arrival position are more spread in ±y and ±x directions respectively as explained in the past slide, hence forming a + sign at the middle
- Like the no-scattering case the ±z valleys electrons are much more spread out as they have less acceleration



Combining effects: Trajectories and Arrival Positions at the Top Surface in Germanium for Each of the Different Valleys Under an Electric Field With Scattering Effects

- Finally, for the Ge case, the Luke scattering causes all the electrons to quickly lose their initial energy and move along the acceleration direction
- Under strong enough voltage (like we have here) the valley-pair arrival points are essentially merged as their initial momentum is not enough to separate them





Summary and Next Steps

- We have described the basics of the charge transportation in a semiconductor crystal
- We have shown the expectations for how each effect would affect what we observe
- We will now move to the pieces that will be included in the full thesis work
- Our ultimate goal is to implement the correct charge transportation physics in the SuperCDMS simulation tool, which uses Geant4
    - To do that, in the full thesis, we will apply special relativity corrections to our charge transportation model to be consistent with Geant4 physics
    - Additionally, as Geant4 does not support anisotropic lattice, we will use the Condensed Matter Physics addon (G4CMP) which does that

Overview of the Geant4 Condensed Matter Physics (G4CMP) Addon

- Since Geant4 does not support anisotropic materials, SuperCMDS uses a custom Geant4 Condensed Matter Physics (G4CMP) addon
  - G4CMP simulates phonon and charge transport in cryogenic semiconductor crystals using the physics we described earlier
  - G4CMP is capable of modeling several physics processes relevant to phonon and charge collection at cryogenic temperatures
  - This add-on allows us to simulate the detector response to both Dark Matter and Standard Model particles
- Additionally, there is a wider use for G4CMP in other fields such as study of qbits to increase the accuracy in the quantum computing
- When we started this project a number of years ago, G4CMP's charge transportation physics did not reflect the physics discussed in this talk, and in some cases was providing results that did not match our expectations

Goal: Implement the correct charge transportation physics in the G4CMP codebase, and verify its results with the expectations we made using the toy model

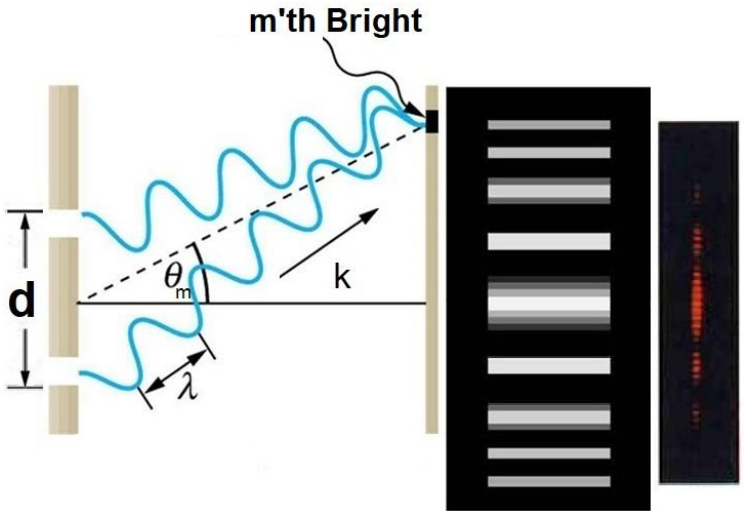
Conclusion

- We have described some of the important components that a high quality detector simulation will need to help SuperCDMS differentiate between Dark Matter and standard model particles
- We provided a basic overview of the charge transportation physics in a semiconductor detector that will be included in the G4CMP add-on which will have impact in both dark matter searches and other fields
- We presented the expectations for the full simulation based on a toy model focusing on the dominant effects of charge transportation in a semiconductor crystal
- The plan for the rest of the thesis work is to implement the charge transportation physics in the SuperCDMS detector simulation

Backup Slides

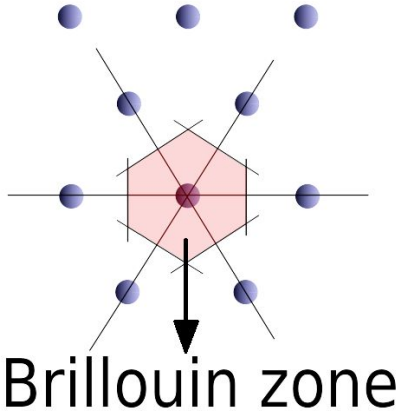
Electron’s Wavevector

- This figure shows a three different views of the famous double-slit experiment, but using electrons.
- The double slit experiment demonstrates that electrons can satisfy the definition of both wave and particle.
- The wavevector, k, can be defined with magnitude $|k|=2\pi/\lambda$ where λ is given by the DeBroglie wave relation as $m\lambda=d\sin\theta_m$ and with the direction of electron wave propagation



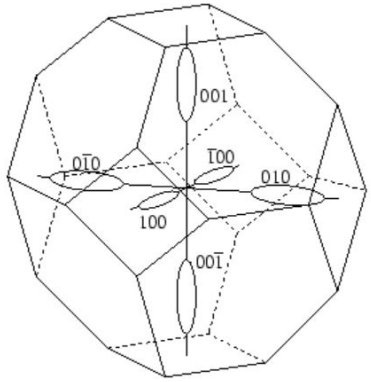
Brillouin Zone

- Bloch's theorem implies that the wavefunctions of the charges in a periodic lattice can be expressed as periodic functions in wavevector space
- This periodicity in wavevector space is called the reciprocal lattice, which is the wavevector space equivalent of the real-space crystal lattice, shown in the figure
- Brillouin zone is a uniquely defined primitive cell in reciprocal space
- The focus of the figure is the first Brillouin zone, the region closer to the origin than any other lattice point
- In crystals with a periodic potential, wave states can be fully described by their behavior within a single Brillouin zone

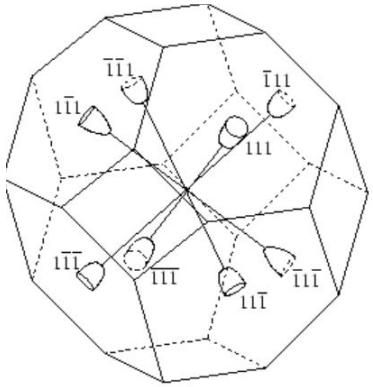


L and X directions in the Brillouin Zone

- These figures show a three diagrams which illustrate the periodic structure of a crystal in the reciprocal lattice of a face-centered cubic (FCC) structure
- Important points in the Brillouin zone of an FCC lattice include the X points at the centers of square faces (top diagram) and the L points at the centers of hexagonal faces (bottom diagram) in which the energy of an electron in conduction band will be minimized
- It turns out that the X points will be the “valleys” directions for silicon and the L points will be the “valleys” directions for germanium



X directions in Brillouin Zone



L directions in Brillouin Zone

Band Gaps for Si and Ge in SuperCDMS Settings

- For Silicon the the lowest conduction band energy level is for charges with a wavevector along the six X directions in the Brillouin Zone and this band gap is equal to:

$$E_g = 0.7437 - \frac{4.77\times10^{-4}T^2}{T+235}\ \text{eV}$$

- For Germanium the the lowest conduction band energy level is for charges with a wavevector along the eight L directions in the Brillouin Zone and this band gap is equal to:

$$E_g = 1.166 - \frac{4.73\times10^{-4}T^2}{T+636}\ \text{eV}$$

- SuperCDMS detectors work at around 50mK temperature, which means a band gap of **1.116eV** for Silicon and a bang gap of **0.7437eV** for Germanium