Terahertz Circular Dichroism Spectroscopy

Who We Are

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Mentor: Jing Xu, UCSB, Physics

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Dr. S. James Allen, UCSB, Physics

Who Funds Us

UCSB, Army, NASA

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What Do We Do?

- Look for a biologically specific phenomena, “circular dichroism”.

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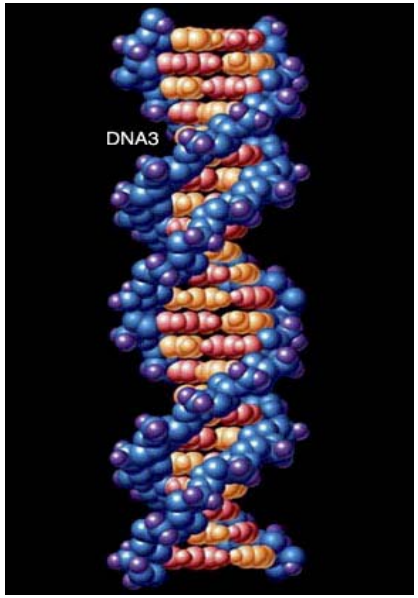
Circular Dichroism: due to interaction between biopolymers and EM radiation.

http://www.rit.edu/~japfaa/molecules.html



Typical Biopolymer

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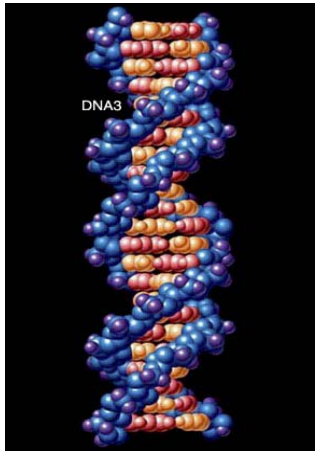
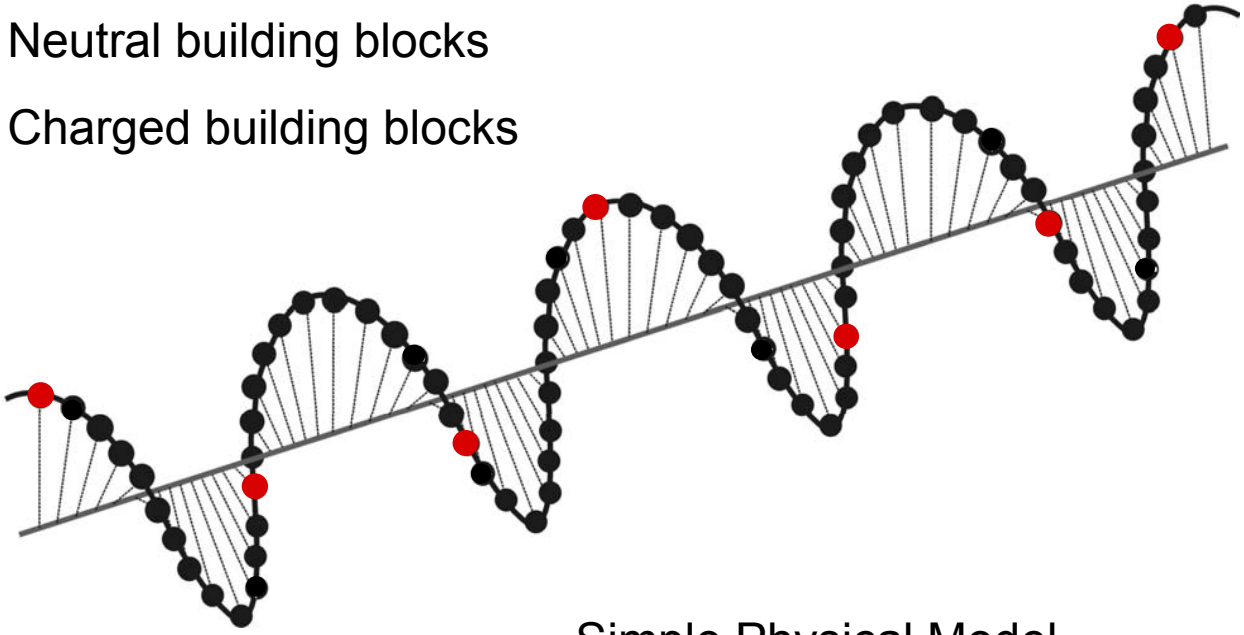
Circular Dichroism: due to interaction between biopolymers and EM radiation.



http://www.rit.edu/~japfaa/molecules.html

Typical Biopolymer

- Neutral building blocks
- Charged building blocks



Simple Physical Model

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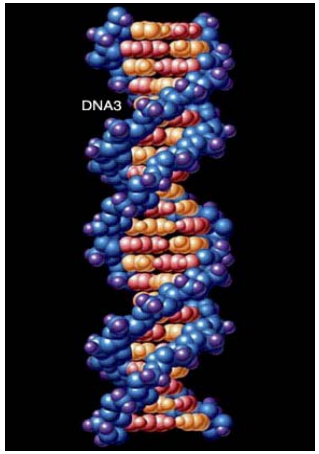
Circular Dichroism: due to interaction between biopolymers and EM radiation.



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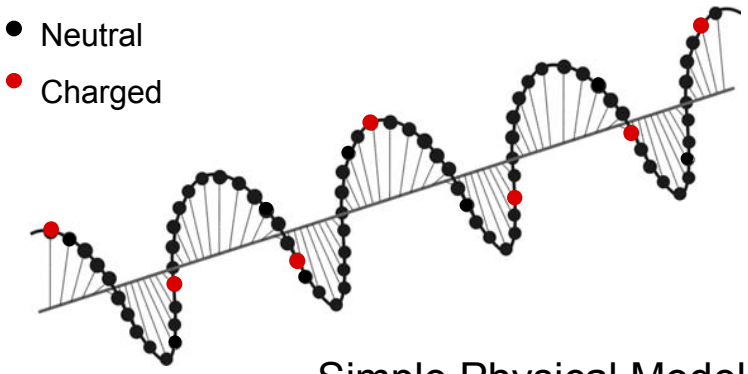
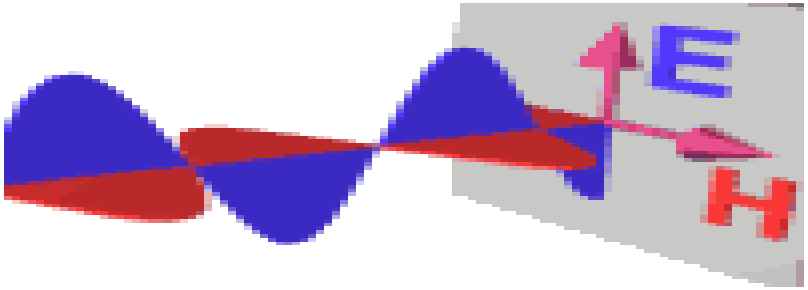


Simple Physical Model

charges move, biopolymers move.



Sample EM Radiation

http://physics.nad.ru/Physics/English/ell_txt.htm

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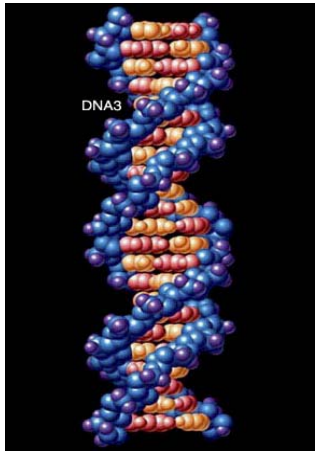
Circular Dichroism: due to interaction between biopolymers and EM radiation.



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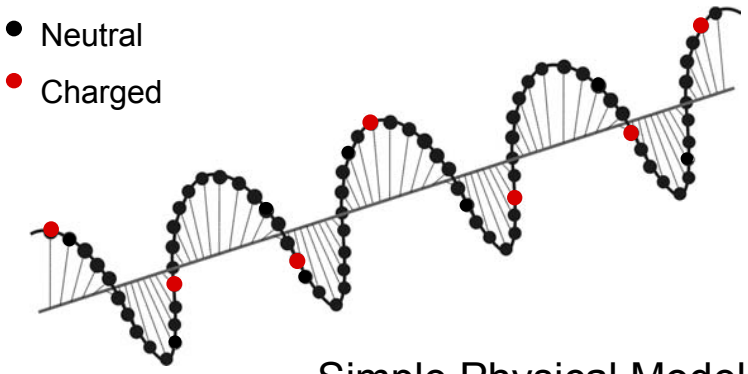
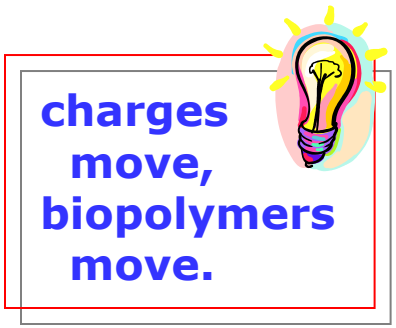
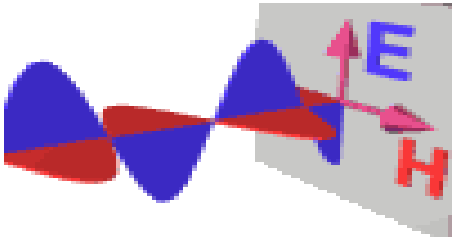
Typical Biopolymer



Simple Physical Model





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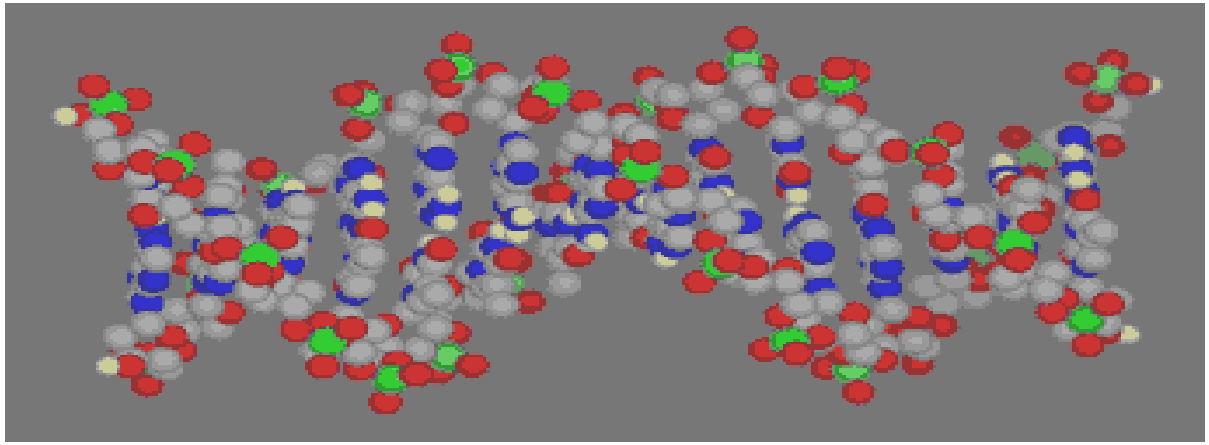

http://projects.villa-bosch.de/dbase/dsmm/

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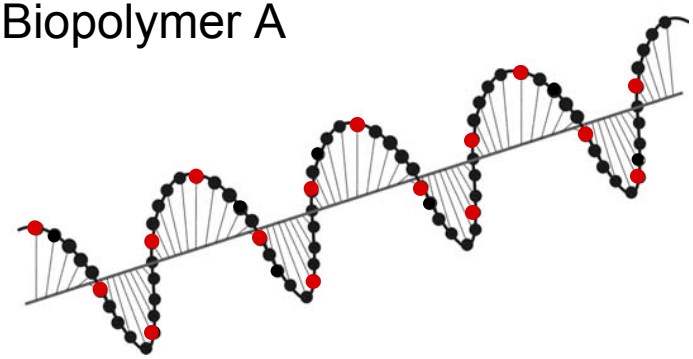
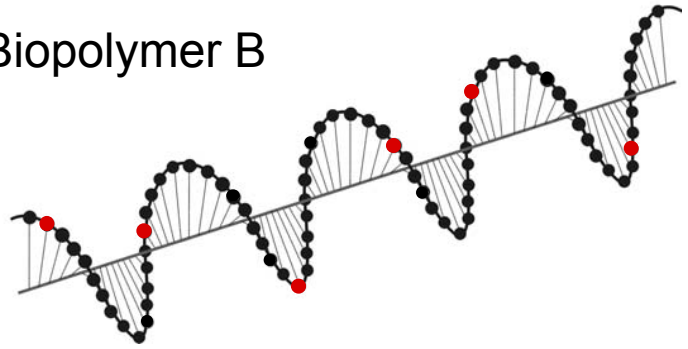
Circular Dichroism: unique to each biopolymer.

Biopolymer A



Biopolymer B



Each Biopolymer has a unique distribution of charged building blocks.

Circular Dichroism produced at any wavelength: Unique to Biopolymer

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What Makes Us Special: Terahertz Circular Dichroism.

- NOT explored before.
- Study large-scale dynamics in biopolymers.

Real time observation of
large-scale protein folding and unfolding (Biochemists)

- Circular dichroism produced at ANY wavelength is
Unique to each biopolymer.

All biopolymers interact with (absorb) Terahertz radiation.

Detection of life (NASA)

Identification of biochemical agents (Army)

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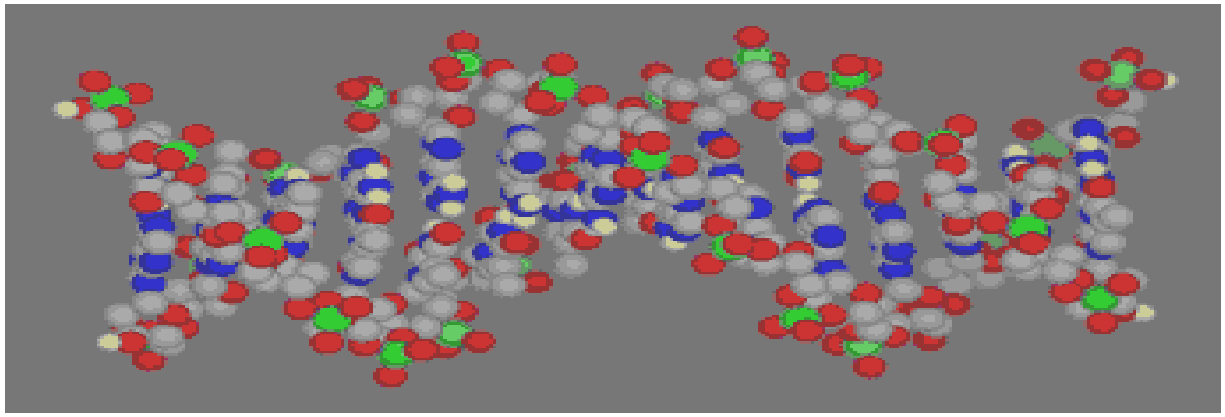
How do we go about modeling the Terahertz Circular Dichorism:

Goal and Approach:

Need information on the trajectory of charged building blocks of biopolymer
in order to
understand the interaction between biopolymer and Terahertz radiation,
in order to
calculate Terahertz Circular Dichroism.

Trajectory

The path of
a moving object
through space
over time.



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How do we go about modeling the Terahertz Circular Dichorism:

Step 1: Need information on the trajectory of charged building blocks.

Step 1 a: Write down equation of motion for each charged building block:

$$\mathbf{I}\cdot\frac{\mathbf{d}^2}{\mathbf{dt}^2}\theta_{\mathbf{i}} = -\alpha\cdot\left(\theta_{\mathbf{i}} - \theta_{\mathbf{i+1}}\right) - \alpha\cdot\left(\theta_{\mathbf{i}} - \theta_{\mathbf{i-1}}\right) + \mathbf{q_i}\cdot\mathbf{b}\cdot\varepsilon_{\mathbf{x}}\cdot\mathbf{e}^{\mathbf{j}\cdot\left(\omega\cdot\mathbf{t}-\mathbf{k}\cdot z_i\right)}\cdot\sin\left(\phi_{\mathbf{i}}\right)$$

Step 1 b: Solve this equation of motion to get the trajectory of all charged building blocks on a biopolymer.

Solving method: analytically: using pencil and paper.

Step 2: Understand the interaction between biopolymer and Terahertz radiation,

Step 3: Calculate Terahertz Circular Dichroism.

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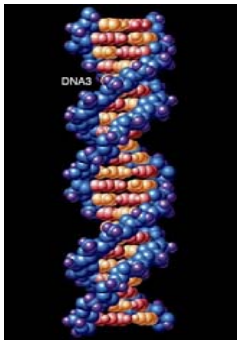
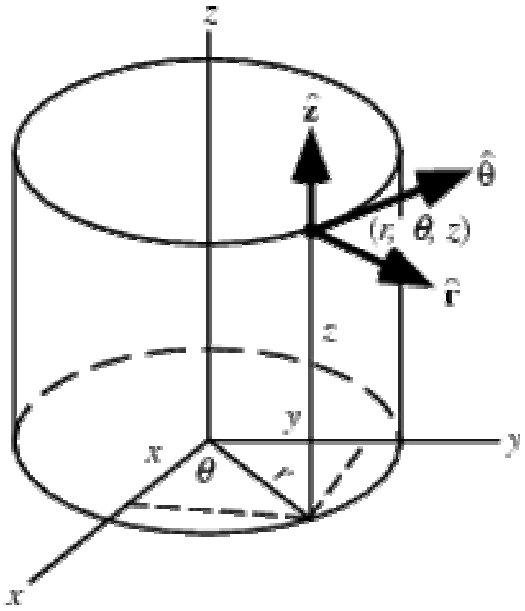
Equation of motion for charged building blocks: cylindrical coordinates: r_i, z_i, θ_i

$$I \cdot \frac{d^2}{dt^2}\theta_i = -\alpha \cdot (\theta_i - \theta_{i+1}) - \alpha \cdot (\theta_i - \theta_{i-1}) + q_i \cdot b \cdot \varepsilon_x \cdot e^{j \cdot (\omega \cdot t - k \cdot z_i)} \cdot \sin(\phi_i)$$





Cylindrical Coordinates:

r, z, θ.

http://mathworld.wolfram.com/CylindricalCoordinates.html

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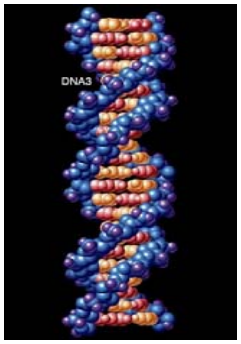
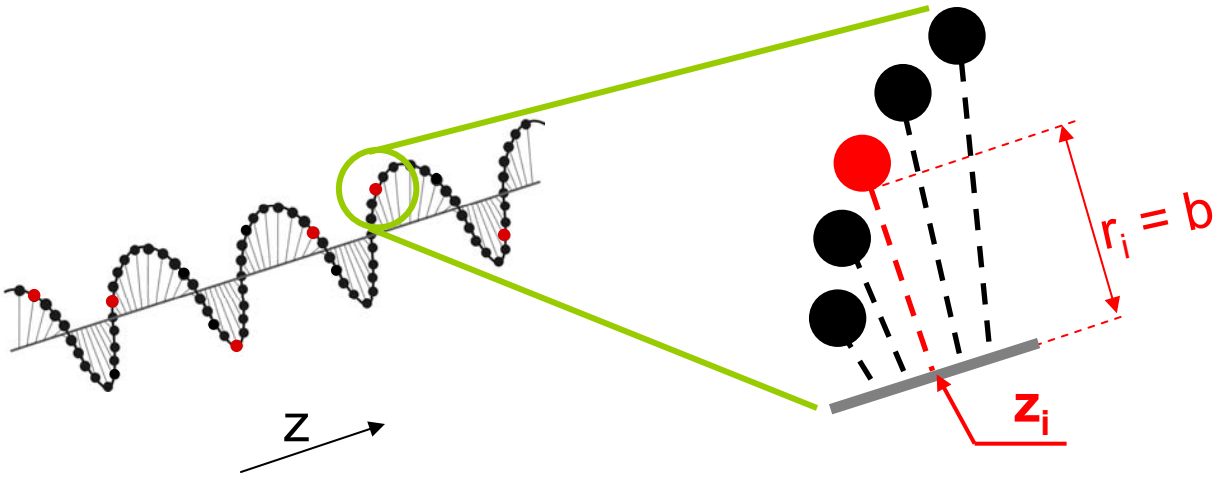
Equation of motion for charged building blocks: cylindrical coordinates: r_i, z_i, θ_i

$$I \cdot \frac{d^2}{dt^2}\theta_i = -\alpha \cdot (\theta_i - \theta_{i+1}) - \alpha \cdot (\theta_i - \theta_{i-1}) + q_i \cdot b \cdot \varepsilon_x \cdot e^{j \cdot (\omega \cdot t - k \cdot z_i)} \cdot \sin(\phi_i)$$





For each charged building block,
we describe their position with $r_i = b$, z_i, θ_i,

where subscript i keeps track each of the charged building blocks.

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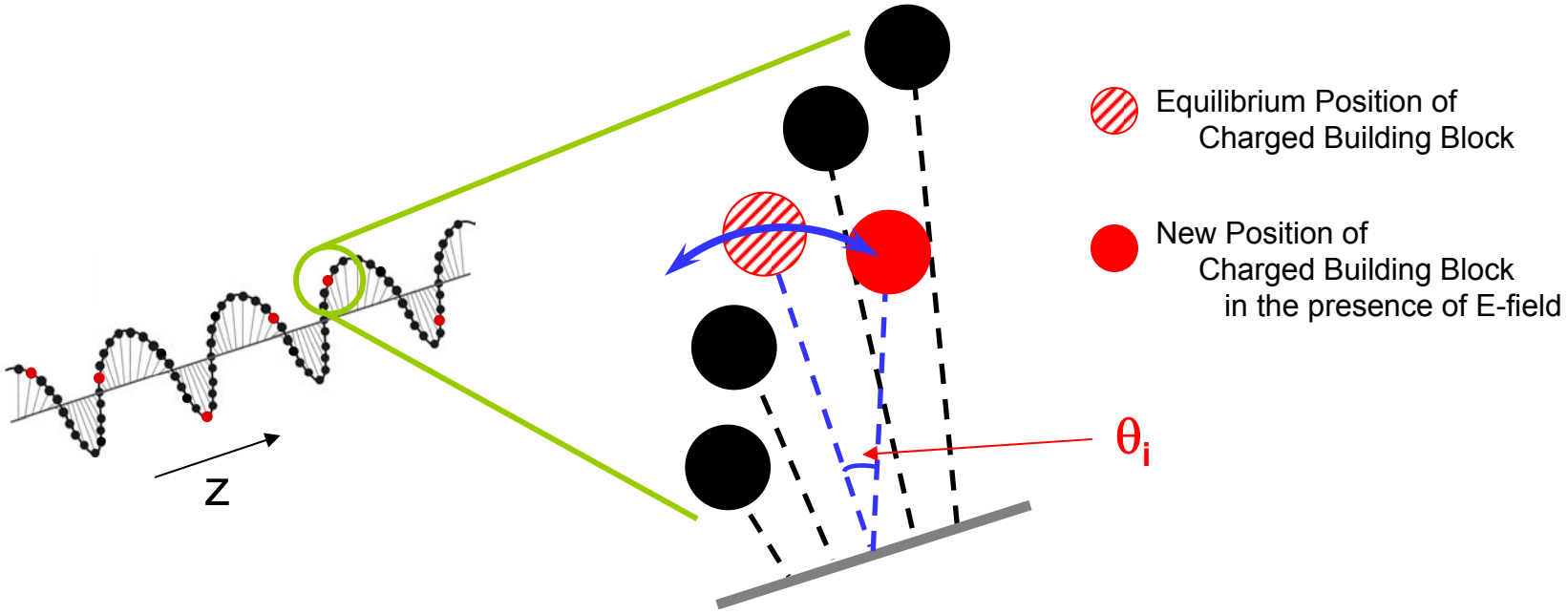
Equation of motion for charged building blocks: cylindrical coordinates: r_i, z_i, θ_i

$$I \cdot \frac{d^2}{dt^2}\theta_i = -\alpha \cdot (\theta_i - \theta_{i+1}) - \alpha \cdot (\theta_i - \theta_{i-1}) + q_i \cdot b \cdot \varepsilon_x \cdot e^{j \cdot (\omega \cdot t - k \cdot z_i)} \cdot \sin(\phi_i)$$



Only movement in the tangential plane to the backbone is allowed.

ϕ_i = equilibrium position. θ_i = displacement from ϕ_i

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Equation of motion for charged building blocks: what it means

$$\mathbf{I}\cdot\frac{\mathbf{d}^2}{\mathbf{dt}^2}\theta_i = -\alpha\cdot\left(\theta_i - \theta_{i+1}\right) - \alpha\cdot\left(\theta_i - \theta_{i-1}\right) + \mathbf{q_i}\cdot\mathbf{b}\cdot\varepsilon_x\cdot\mathbf{e}^{\mathbf{j}\cdot\left(\omega\cdot\mathbf{t}-\mathbf{k}\cdot z_i\right)}\cdot\sin\left(\phi_i\right)$$

Recipe for writing down the equation of motion of a particle:

mass * acceleration = all forces experienced

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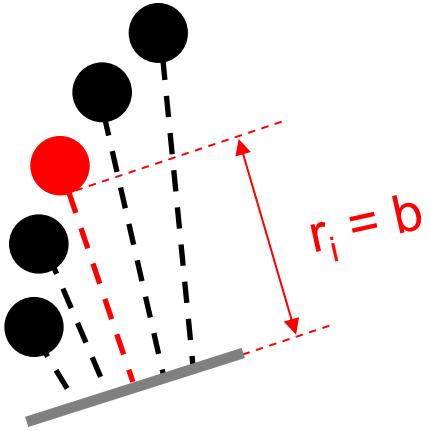
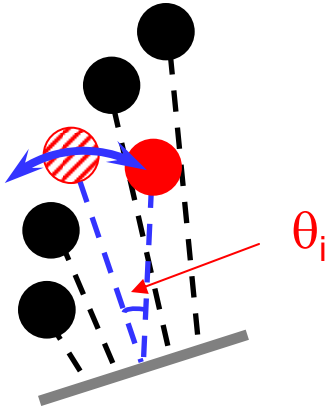
Equation of motion for charged building blocks: left hand side

$$I \cdot \frac{d^2}{dt^2}\theta_i = -\alpha \cdot (\theta_i - \theta_{i+1}) - \alpha \cdot (\theta_i - \theta_{i-1}) + q_i \cdot b \cdot \varepsilon_x \cdot e^{j \cdot (\omega \cdot t - k \cdot z_i)} \cdot \sin(\phi_i)$$





I = Inertia of the charged building block = mass * b^2 ~ mass

$\frac{d^2}{dt^2}\theta_i$ = second derivative of displacement angle = acceleration

LHS = mass * acceleration

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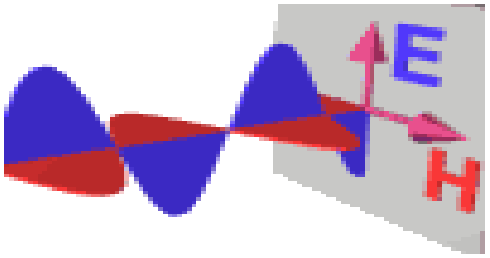
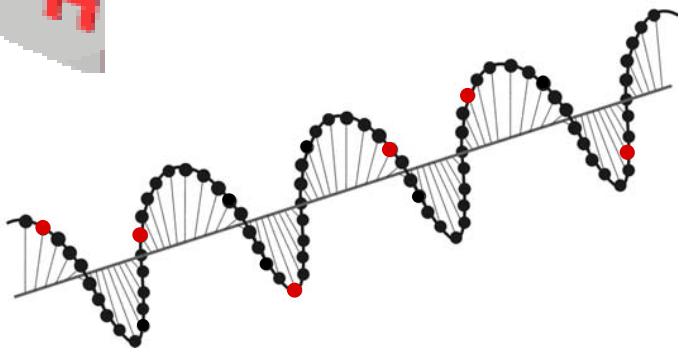
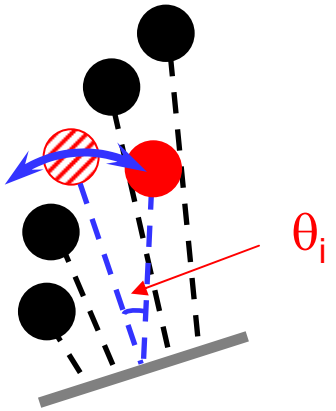
Equation of motion for charged building blocks: right hand side

$$I \cdot \frac{d^2}{dt^2}\theta_i = -\alpha \cdot (\theta_i - \theta_{i+1}) - \alpha \cdot (\theta_i - \theta_{i-1}) + q_i \cdot b \cdot \varepsilon_x \cdot e^{j \cdot (\omega \cdot t - k \cdot z_i)} \cdot \sin(\phi_i)$$

Force experienced by each charged units due to external terahertz radiation.







Terahertz radiation shakes and pushes each charged units around.

Each charged units can only move in the tangential plane to the backbone.

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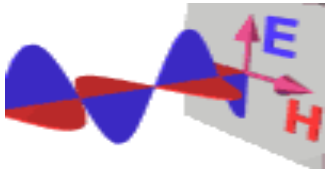
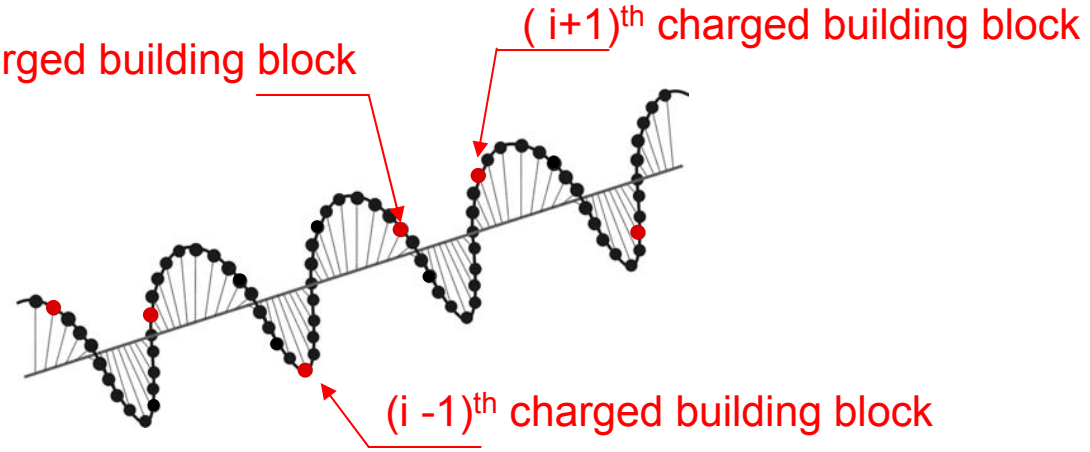
Equation of motion for charged building blocks: right hand side

$$I \cdot \frac{d^2}{dt^2}\theta_i = -\alpha \cdot (\theta_i - \theta_{i+1}) - \alpha \cdot (\theta_i - \theta_{i-1}) + q_i \cdot b \cdot \varepsilon_x \cdot e^{j \cdot (\omega \cdot t - k \cdot z_i)} \cdot \sin(\phi_i)$$

Force experienced due to the motions of the two closest charged neighbors.





α = "coupling strength between closest charged neighbors".

Movements of an individual charged unit

can and do also cause the two closest neighbors to move.

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Equation of motion for charged building blocks: right hand side

$$\mathbf{I}\cdot\frac{d^2}{dt^2}\theta_i = -\alpha\cdot(\theta_i-\theta_{i+1})-\alpha\cdot(\theta_i-\theta_{i-1}) + q_i\cdot b\cdot\varepsilon_x\cdot e^{j\cdot(\omega\cdot t-k\cdot z_i)}\cdot\sin(\phi_i)$$

Force experienced by each charged units due to external terahertz radiation.

Force experienced due to the motions of the two closest charged neighbors.

RHS = all forces experienced by a single charged building block

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Equation of motion for charged building blocks: the whole thing

$$I \cdot \frac{d^2}{dt^2}\theta_i = -\alpha \cdot (\theta_i - \theta_{i+1}) - \alpha \cdot (\theta_i - \theta_{i-1}) + q_i \cdot b \cdot \varepsilon_x \cdot e^{j \cdot (\omega \cdot t - k \cdot z_i)} \cdot \sin(\phi_i)$$

Force experienced by each charged units due to external terahertz radiation.

Force experienced due to the motions of the two closest charged neighbors.

Mass * acceleration.

How do we go about solving it?

Quick Answer: use more pencil and paper.

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Acknowledgements:

Mentor	Faculty Advisors	INSET	Sponsors
➢Jing Xu	➢Dr. Kevin W. Plaxco	➢DR. Arnold	➢INSET
	➢Dr. S. James Allen	➢Trevor Hirst	➢CNSI
		➢Mike Northern	➢NSF
			➢UCSB
			➢NASA
			➢ARMY

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➢ Thank You MESA (Allan Hancock College)