Introduction to Molecular Spectroscopy

Fundamental Concepts in Spectroscopy and Electrodynamics

Mike Reppert

August 21, 2019

Outline for Today:

1. Syllabus
2. Introduction to Spectroscopy and Electrodynamics
   - What is spectroscopy?
   - What is the Electromagnetic Field?
     - The field as a force map
     - The field as a flow map
     - The field as a propagating wave

Syllabus

Web Page

https://mreppert.github.io/education/chm676/index.html

Introduction to Spectroscopy and Electrodynamics

What is Spectroscopy?

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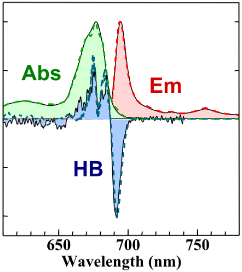
A few examples:

Linear(ish)



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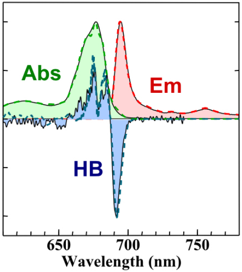
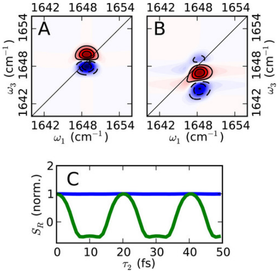


Multidimensional



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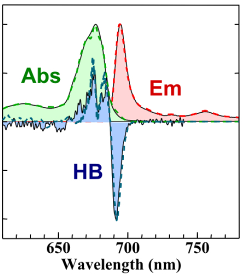

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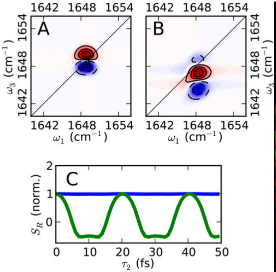
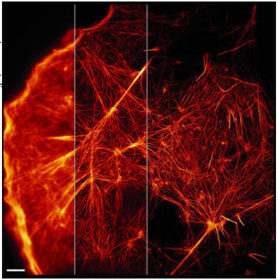


Imaging



STORM Image Credit:
`www.sciencemag.org/features/2016/05/superresolution-microscopy`

What is the Electromagnetic field?

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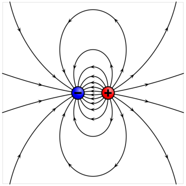
A Force Map:

The **electric field** $e(\boldsymbol{r})$ describes the hypothetical force experienced by a *stationary* particle with infinitesimal charge at location $\boldsymbol{r}$.



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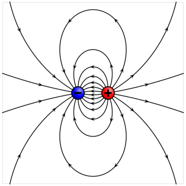

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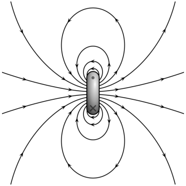

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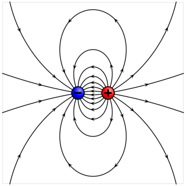

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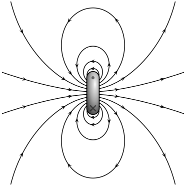
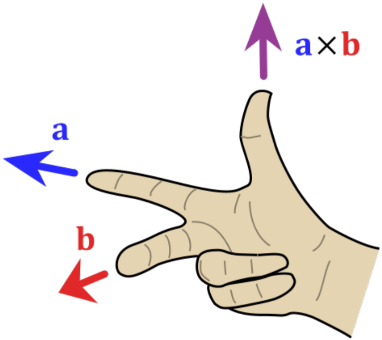


The Lorentz Force Law:

$$\boldsymbol{F}_{EM} = q\left(\boldsymbol{e}(\boldsymbol{r},t) + \frac{\boldsymbol{v}}{c} \times \boldsymbol{b}(\boldsymbol{r},t)\right).$$

The Cross Product

Right-hand Rule



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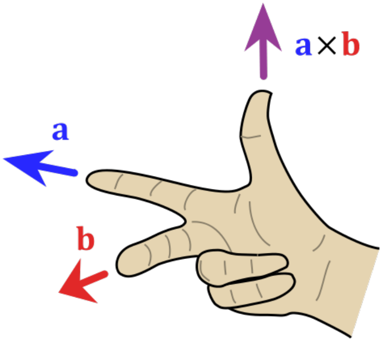


Cyclotron

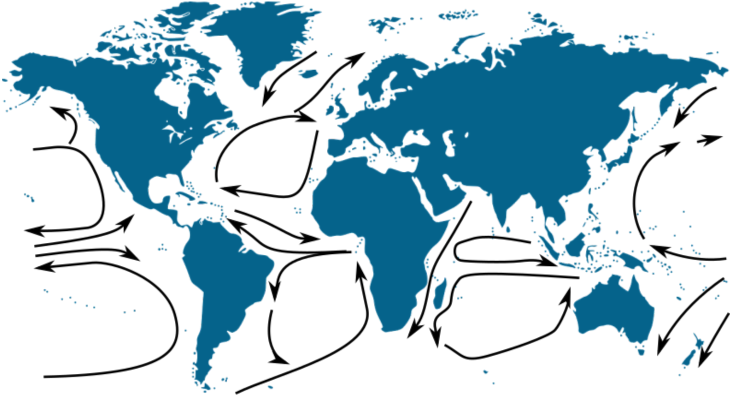
RHR image credit: https://commons.wikimedia.org/wiki/File:Right_hand_rule_cross_product.svg

Cyclotron image credit:
https://blogs.plos.org/thestudentblog/2016/02/26/lawrence/

What is the Electromagnetic field?

A Flow Map:

The electric (magnetic) field can be interpreted as the *velocity field* for a fictitious electrical (magnetic) "substance."



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A Flow Map:

Gauss's Law says that the total flow rate of electrical fluid *out of* any closed surface is proportional to the total charge *enclosed by* the surface.

$$\nabla \cdot \boldsymbol{e} \equiv \frac{\partial e_x}{\partial x} + \frac{\partial e_y}{\partial y} + \frac{\partial e_z}{\partial z} = 4\pi\varrho(\boldsymbol{x}, t)$$

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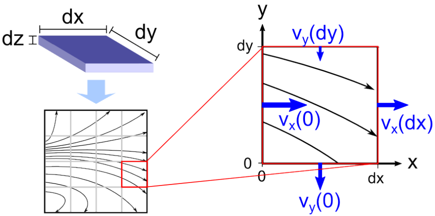

In two dimensions:

$$\nabla \cdot \boldsymbol{v} \sim \frac{dv_x}{dx} + \frac{dv_y}{dy}$$

What is the Electromagnetic field?

A Flow Map:

The **Maxwell-Faraday Equation** says that temporal changes in the magnetic field produce "swirls" in the electric field.

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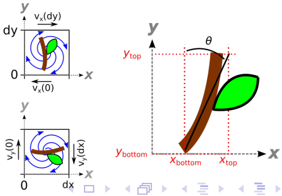
$$\nabla \times \boldsymbol{v} = \begin{vmatrix} \hat{\boldsymbol{x}} & \hat{\boldsymbol{y}} & \hat{\boldsymbol{z}} \\ \frac{\partial}{\partial x} & \frac{\partial}{\partial y} & \frac{\partial}{\partial z} \\ v_x & v_y & v_z \end{vmatrix}$$



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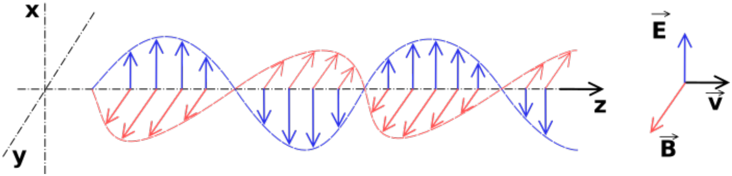
A Propagating Wave:

According to Maxwell's equations:

- A changing E-field creates a B-field
- A changing B-field creates an E-field...

...self-propagation!



Infinities in Field-Particle Interactions

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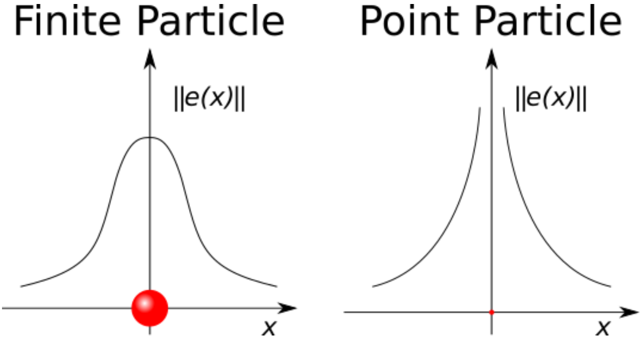

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Okay for point-particles:

$$\boldsymbol{F}_{\text{EM}} = q\left(\boldsymbol{e}^{(\text{eff})} + \frac{\boldsymbol{v}}{c} \times \boldsymbol{b}(\boldsymbol{r})\right),$$

where

$$\boldsymbol{e}^{(\text{eff})} = \lim_{\boldsymbol{r}' \to \boldsymbol{r}} \left(\boldsymbol{e}(\boldsymbol{r}') - q\frac{\boldsymbol{r}}{|\boldsymbol{r}' - \boldsymbol{r}|^2}\right)$$