

Introduction to Molecular Spectroscopy

Fundamental Concepts in Spectroscopy and Electrodynamics

Mike Reppert

August 19, 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](https://mreppert.github.io/education/chm676/index.html)

Introduction to Spectroscopy and Electrodynamics

What is Spectroscopy?

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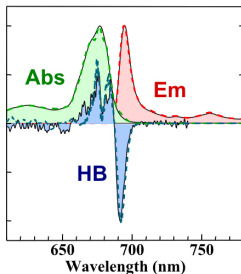
Spectroscopy: *The study of the interaction of light and matter*

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A few examples:

Linear(ish)

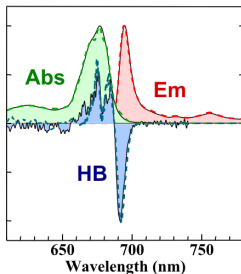


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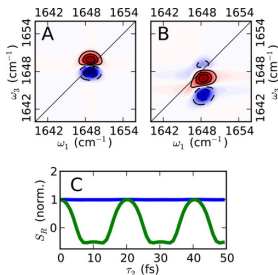
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Multidimensional

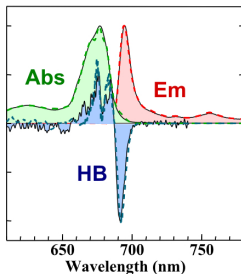


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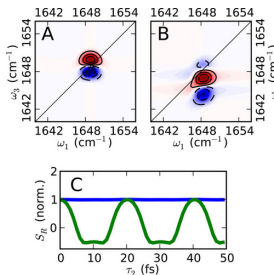
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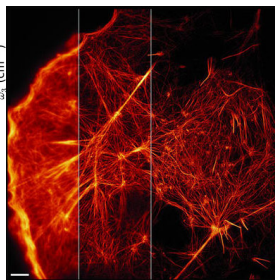
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Multidimensional



Imaging



STORM Image Credit:

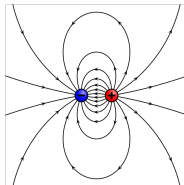
www.sciencemag.org/features/2016/05/superresolution-microscopy

What is the Electromagnetic field?

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A Force Map:

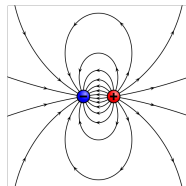
The **electric field** $e(\mathbf{r})$ describes the hypothetical force experienced by a *stationary* particle with infinitesimal charge at location \mathbf{r} .



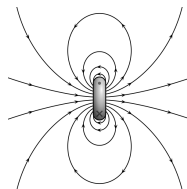
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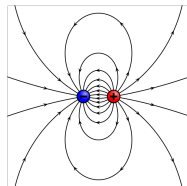
The **magnetic field** $b(\mathbf{r})$ describes the *additional* hypothetical force experienced by a *moving* particle with infinitesimal charge at location \mathbf{r} .



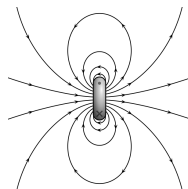
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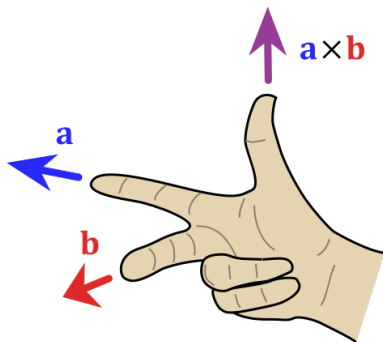


The Lorentz Force Law:

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

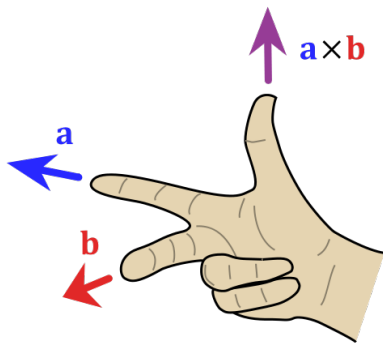
The Cross Product

Right-hand Rule



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Right-hand Rule



Cyclotron



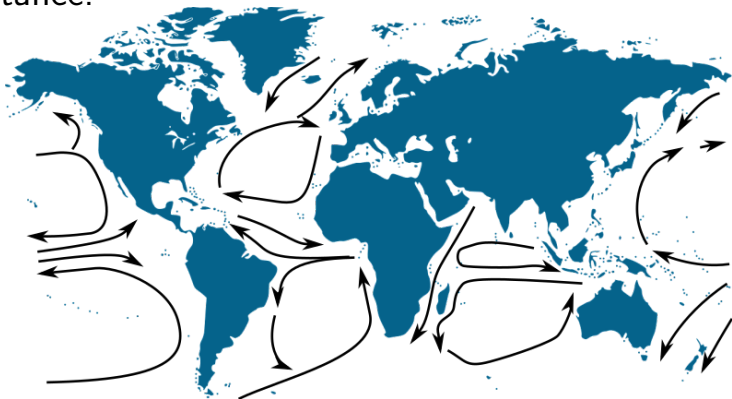
RHR image credit: https://commons.wikimedia.org/wiki/File:Right_hand_rule_cross_product.svg

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.”



What is the Electromagnetic field?

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.

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

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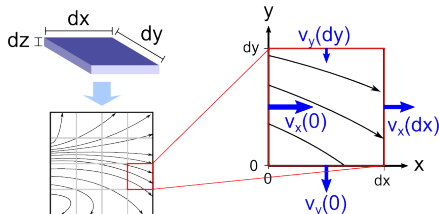
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In two dimensions:

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

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.

$$\nabla \times \mathbf{e} + \frac{1}{c} \frac{\partial \mathbf{b}}{\partial t} = 0$$

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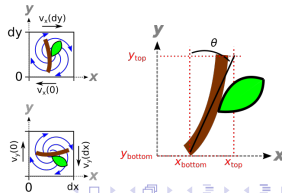
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$$\nabla \times \mathbf{v} = \begin{vmatrix} \hat{\mathbf{x}} & \hat{\mathbf{y}} & \hat{\mathbf{z}} \\ \frac{\partial}{\partial x} & \frac{\partial}{\partial y} & \frac{\partial}{\partial z} \\ v_x & v_y & v_z \end{vmatrix}$$



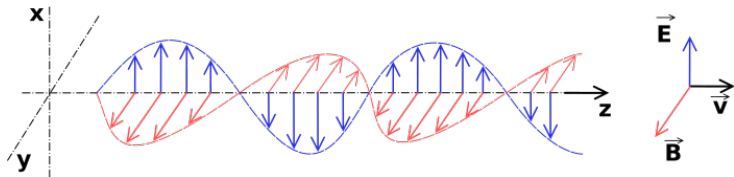
What is the Electromagnetic field?

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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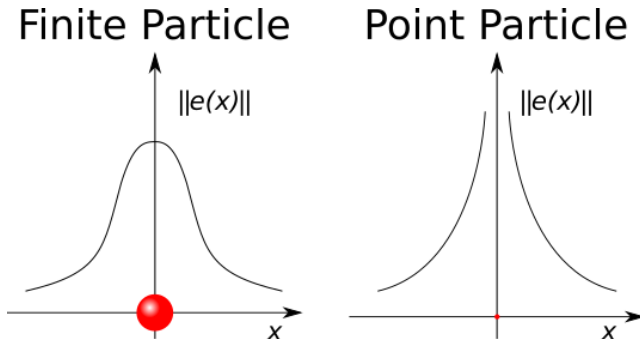
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The electric field always diverges in the vicinity of point particles



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Okay for point-particles:

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

where

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