Introduction to Molecular Spectroscopy

Fundamental Concepts in Spectroscopy and Electrodynamics

Mike Reppert

Outline for Today:

1. 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

Introduction to Spectroscopy and Electrodynamics

What is Spectroscopy?

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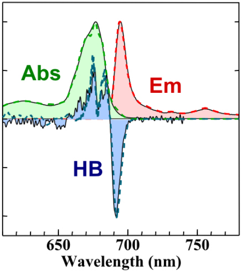
A few examples:

Linear(ish)



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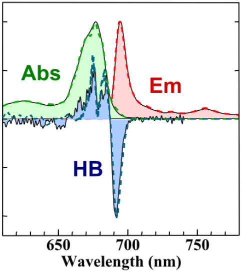
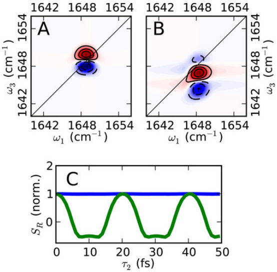


Multidimensional



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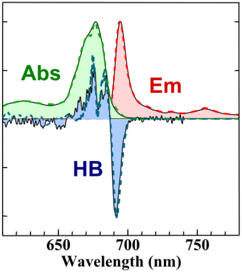

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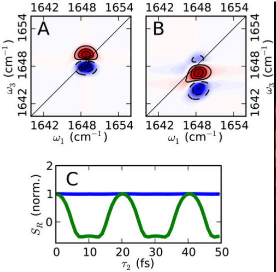
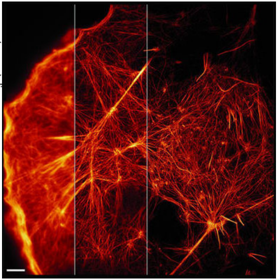


Imaging



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

What is the Electromagnetic field?

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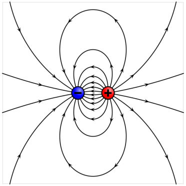
A Force Map:

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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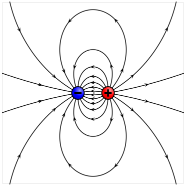

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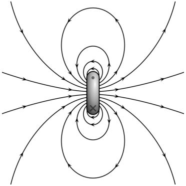

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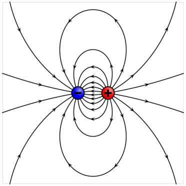

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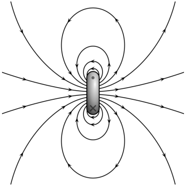
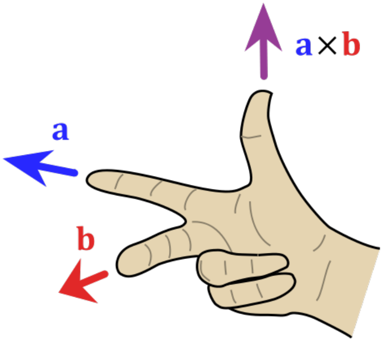


The Lorentz Force Law:

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

The Cross Product

Right-hand Rule



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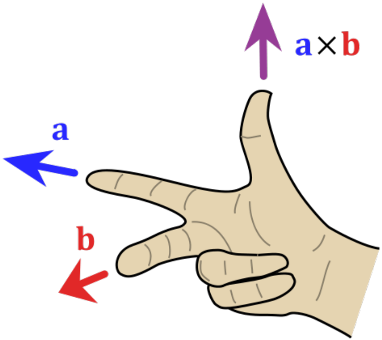

Cyclotron

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/`

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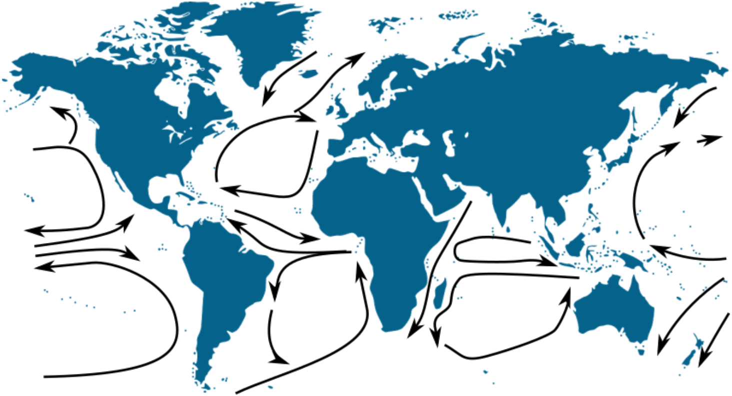
A Flow Map:

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



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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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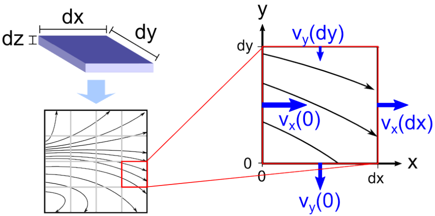

In two dimensions:

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

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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$$= \left(\frac{\partial v_z}{\partial y} - \frac{\partial v_y}{\partial z}\right)\hat{\boldsymbol{x}} - \left(\frac{\partial v_z}{\partial x} - \frac{\partial v_x}{\partial z}\right)\hat{\boldsymbol{y}} + \left(\frac{\partial v_y}{\partial x} - \frac{\partial v_x}{\partial y}\right)\hat{\boldsymbol{z}}$$

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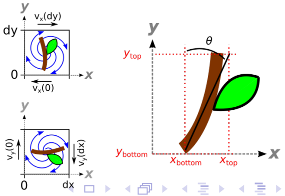

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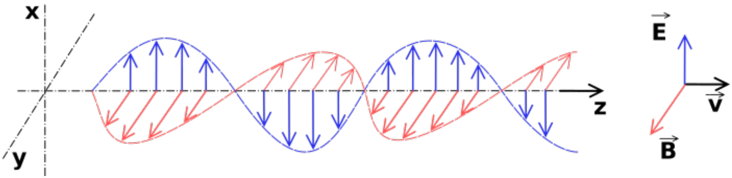
A Propagating Wave:

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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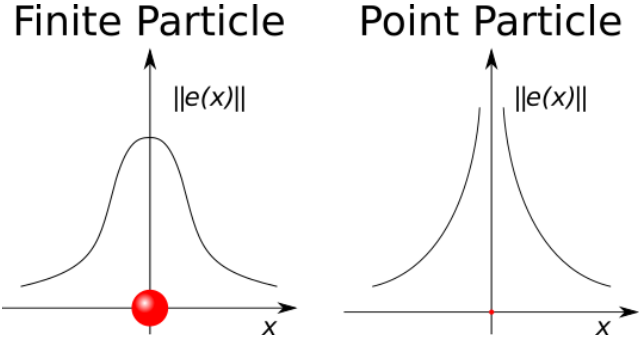
The electric field always diverges in the vicinity of point particles



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Okay for point-particles:

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

where

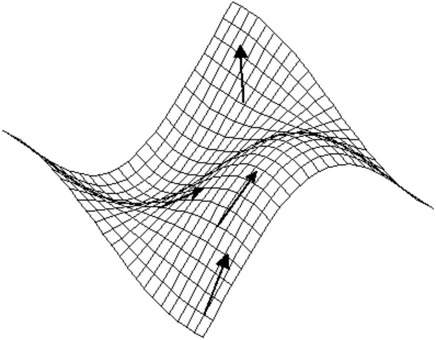
$$\boldsymbol{e}^{(\mathsf{eff})} = \lim_{\boldsymbol{r}' \to \boldsymbol{r}} \left(\boldsymbol{e}(\boldsymbol{r}') - q\frac{\boldsymbol{r}}{|\boldsymbol{r}' - \boldsymbol{r}|^2}\right)$$

Vector Operators

The **gradient** of a *scalar* function is a *vector*

$$\nabla f(\boldsymbol{x}) = \left(\frac{\partial f}{\partial x}, \frac{\partial f}{\partial y}, \frac{\partial f}{\partial z}\right) \tag{1}$$

that points in the direction of *maximum increase* of $f(\boldsymbol{x})$.

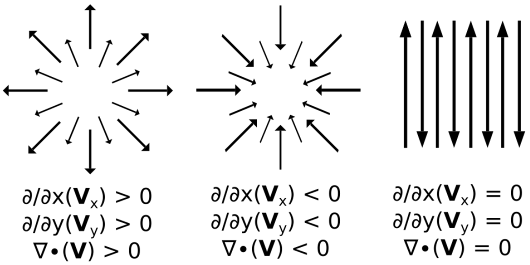


Vector Operators

The **divergence** of a **vector** function is a *scalar*

$$\nabla \cdot \boldsymbol{v}(\boldsymbol{x}) = \frac{\partial \boldsymbol{v}}{\partial x} + \frac{\partial \boldsymbol{v}}{\partial y} + \frac{\partial \boldsymbol{v}}{\partial z} \tag{2}$$

that (if $\boldsymbol{v}$ may be interpreted as a fluid flow field) indicates *how much fluid* flows into or out of a given point.



https://en.wikipedia.org/wiki/Divergence

Vector Operators

The **curl** of a **vector** function is a *vector*

$$\nabla \times \boldsymbol{v}(\boldsymbol{x}) = \begin{vmatrix} \hat{\boldsymbol{x}} & \hat{\boldsymbol{y}} & \hat{\boldsymbol{z}} \\ \frac{\partial}{\partial x} & \frac{\partial}{\partial y} & \frac{\partial}{\partial z} \\ v_x & v_y & v_z \end{vmatrix} \tag{3}$$

that (if $\boldsymbol{v}$ may be interpreted as a fluid flow field) indicates *how strongly the fluid circulates* around a given point in space.