PHY 712 Electrodynamics
11-11:50 AM MWF Olin 107

Plan for Lecture 15:

Finish reading Chap. 5, start Chap. 6

A. Magnetic susceptibility

B. Magnetic boundary value problems

C. Effects of time varying fields and sources

Course schedule for 2013

(Preliminary schedule -- subject to frequent adjustment.)

	Date	JDJ Reading	Topic	Assign.
1	01-16(Wed)	Chap. 1	Introduction, units and Poisson equation.	#1
2	01-18(Fri)	Chap. 1	Electronstatic energy calculations	#2
	01-21(Mon)	*No class*	*MKL Holiday*	
3	01-23(Wed)	Chap. 1	Poisson Equation and Green's Functions	#3
4	01-25(Fri)	Chap. 1 & 2	Green's Theorem and Functions	#4
5	01-28(Mon)	Chap. 1 & 2	Brief introduction to numerical methods	#5
6	01-30(Wed)	Chap. 2	Method of images	#6
7	02-01(Fri)	Chap. 3	Cylindrical and spherical geometries	#7
8	02-04(Mon)	Chap. 4	Multipole moments	#8
9	02-06(Wed)	Chap. 4	Dipoles and dielectrics	#9
10	02-08(Fri)	Chap. 4	Microscopic and macroscopic polarizability	
11	02-11(Mon)	Chap. 5	Magnetostatics	#10
12	02-13(Wed)	Chap. 5	Magnetostatic fields	
13	02-15(Fri)	Chap. 5	Magnetic dipole fields	Exam
14	02-18(Mon)	Chap. 5	Permeable media	Exam
15	02-20(Wed)	Chap. 5	Magnetic susceptibility and permeability	Exam
16	02-22(Fri)	Chap. 6	Maxwell's equations	Exam

WFU Physics Colloquium

TITLE: Needle in a Haystack: Sifting through Predicted Protein Structures for Good Folds

SPEAKER: Professor Xiuping Tao,

Department of Chemistry/Physics,
Winston-Salem State University, Winston-Salem, North Carolina

TIME: Wednesday February 20, 2013 at 4:00 PM

PLACE: Room 101 Olin Physical Laboratory

Refreshments will be served at 3:30 PM in the Olin Lounge. All interested persons are cordially invited to attend.

ABSTRACT

Of the large number of sequence-solved proteins, only a small percentage are structure-solved. It makes protein structure prediction importance. Tremendous computational prediction efforts are applied to generate possible protein structures (decoys), often thousands or even millions of them, for a given sequence. Identifying good (near-native) structures among them can be tough. While the RMSD clustering method is often used to do the job, we propose a new method based on clustering amino-acid contacts in decoys. A comparison between our results and those in a CASP (Critical Assessment of protein Structure Prediction) experiment will be presented.

Summary of equations of magnetostatics :

$$\nabla \times \mathbf{B}(\mathbf{r}) = \mu_0 \mathbf{J}_{total}(\mathbf{r})$$

$$\nabla \times \mathbf{H}(\mathbf{r}) = \mathbf{J}_{free}(\mathbf{r})$$

$$\mathbf{B}(\mathbf{r}) = \mu_0 \left(\mathbf{H}(\mathbf{r}) + \mathbf{M}(\mathbf{r})\right)$$

$$\nabla \cdot \mathbf{B}(\mathbf{r}) = 0$$

For the case that $\mathbf{J}_{free}(\mathbf{r})$:

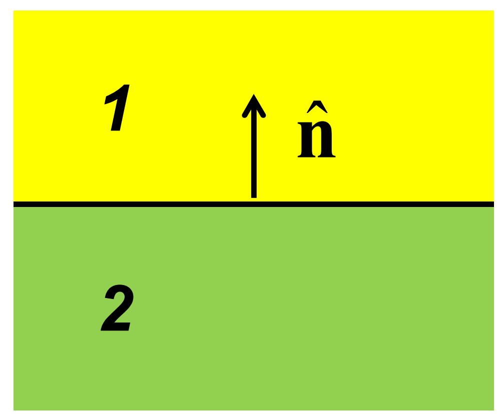
$$\nabla \times \mathbf{H}(\mathbf{r}) = 0$$

$$\nabla \cdot \mathbf{B}(\mathbf{r}) = 0$$

At boundary :

$$\mathbf{H}_1 \times \hat{\mathbf{n}} = \mathbf{H}_2 \times \hat{\mathbf{n}}$$

$$\mathbf{B}_1 \cdot \hat{\mathbf{n}} = \mathbf{B}_2 \cdot \hat{\mathbf{n}}$$



Magnetism in materials

$$\mathbf{B}(\mathbf{r}) = \mu_0(\mathbf{H}(\mathbf{r}) + \mathbf{M}(\mathbf{r}))$$

For materials with linear magnetism:

$$\mathbf{B} = \mu\mathbf{H}$$

$$\mu > \mu_0 \quad \Rightarrow \text{paramagnetic material}$$

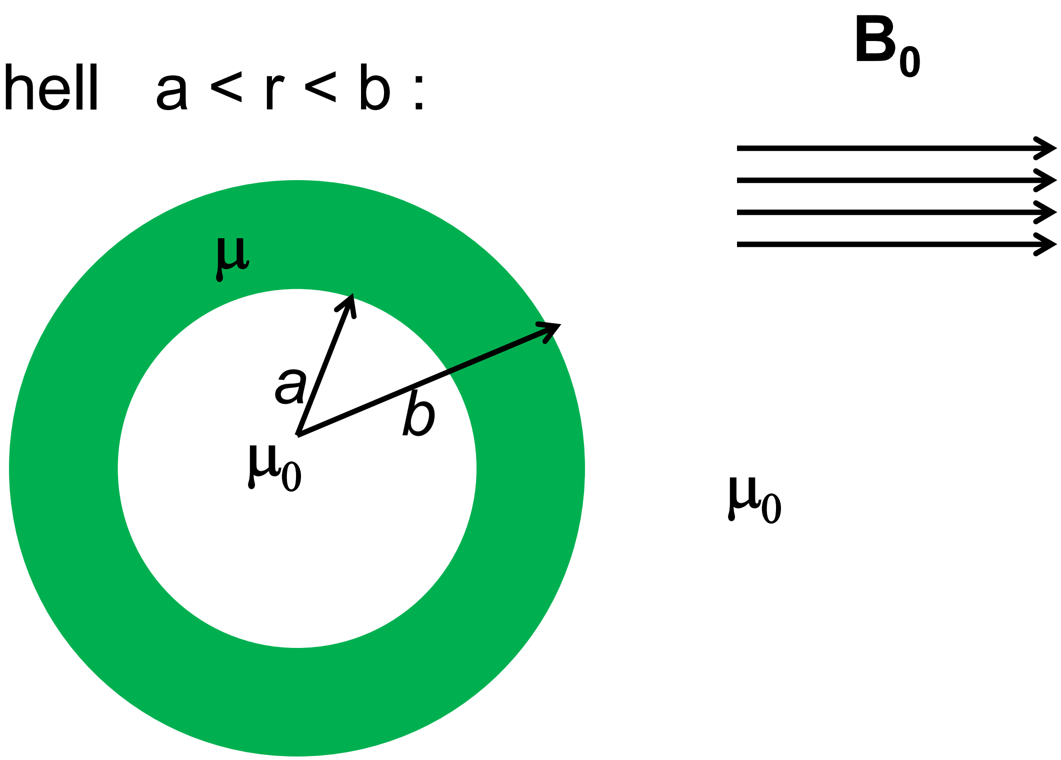
$$\mu < \mu_0 \quad \Rightarrow \text{diamagnetic material}$$

For ferromagnetic, antiferromagnetic materials

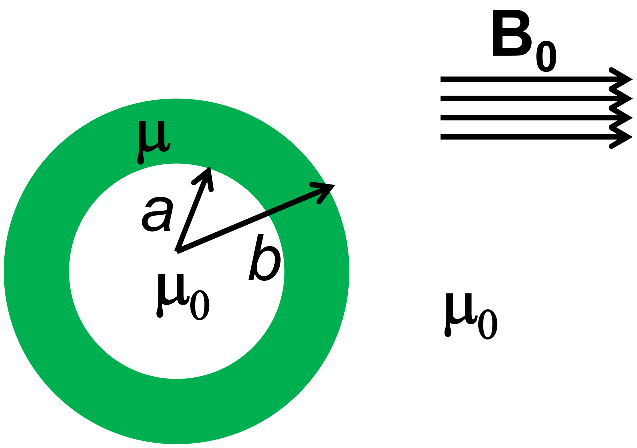
$$\mathbf{B} = f(\mathbf{H}) \quad \text{(with hysteresis)}$$

Example: permalloy, mumetal $\mu/\mu_0 \sim 10^4$

Spherical shell $a < r < b$:



Example: permalloy, mumetal $\mu/\mu_0 \sim 10^4$ -- continued



For this case:

$$\nabla \times \mathbf{H}(\mathbf{r}) = 0$$

$$\nabla \cdot \mathbf{B}(\mathbf{r}) = 0$$

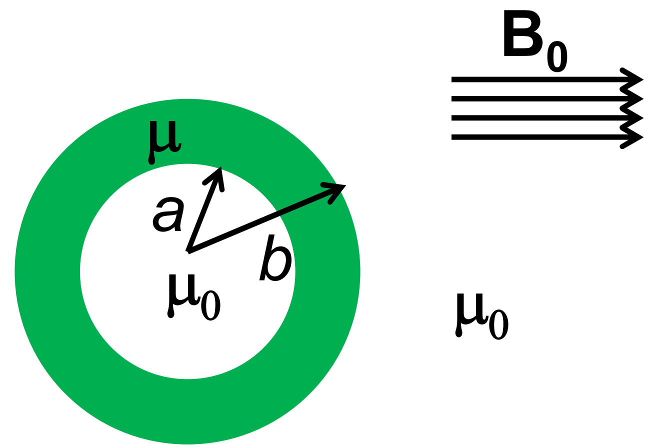
$$\mathbf{B}(\mathbf{r}) = \mu \mathbf{H}(\mathbf{r})$$

Continuity at boundaries:

$$\mathbf{H} \times \hat{\mathbf{n}} = \text{continuous}$$

$$\mathbf{B} \cdot \hat{\mathbf{n}} = \text{continuous}$$

Example: permalloy, mumetal $\mu/\mu_0 \sim 10^4$ -- continued



$$\text{Let:} \quad \mathbf{H}(\mathbf{r}) = -\nabla\Phi_H(\mathbf{r})$$

$$\nabla \cdot \mathbf{B}(\mathbf{r}) = 0 \qquad \Rightarrow \nabla^2\Phi_H(\mathbf{r}) = 0$$

$$\text{For} \quad 0 \leq r \leq a \qquad \Phi_H(\mathbf{r}) = \sum_l \delta_l r^l P_l(\cos\theta)$$

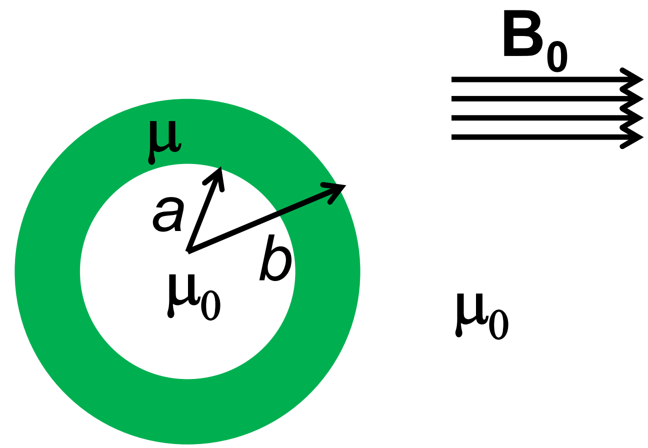
$$\text{For} \quad a \leq r \leq b \qquad \Phi_H(\mathbf{r}) = \sum_l \left(\beta_l r^l + \frac{\gamma_l}{r^{l+1}} \right) P_l(\cos\theta)$$

$$\text{For} \quad r \geq b \qquad \Phi_H(\mathbf{r}) = -\frac{B_0}{\mu_0} r\cos\theta + \sum_l \frac{\alpha_l}{r^{l+1}} P_l(\cos\theta)$$

Example: permalloy, mumetal $\mu/\mu_0 \sim 10^4$ -- continued

Applying boundary conditions

(only $l = 1$ terms contribute):



At $r = a$

$$\delta_1 = \frac{\mu}{\mu_0}\left(\beta_1 - 2\frac{\gamma_1}{a^3}\right)$$

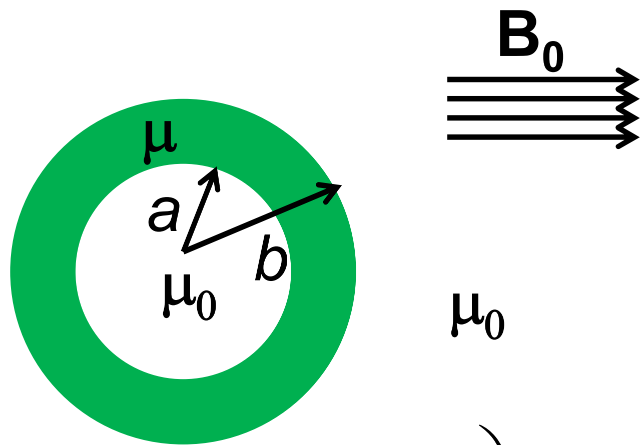
$$a\delta_1 = a\beta_1 + \frac{\gamma_1}{a^2}$$

At $r = b$

$$\frac{\mu}{\mu_0}\left(\beta_1 - 2\frac{\gamma_1}{b^3}\right) = -\frac{B_0}{\mu_0} - 2\frac{\alpha_1}{b^3}$$

$$b\beta_1 + \frac{\gamma_1}{b^2} = -b\frac{B_0}{\mu_0} + \frac{\alpha_1}{b^2}$$

Example: permalloy, mumetal $\mu/\mu_0 \sim 10^4$ -- continued



When the dust clears:

$$\delta_1 = \left(\frac{-9\mu/\mu_0}{(2\mu/\mu_0+1)(\mu/\mu_0+2) - 2(a/b)^3(\mu/\mu_0-1)^2} \right) \frac{B_0}{\mu_0}$$

$$\approx \frac{1}{\mu/\mu_0} \left(\frac{-9/2}{\left(1-(a/b)^3\right)} \frac{B_0}{\mu_0} \right)$$

Energy associated with magnetic fields

Note: We previously used without proof --

the force on a magnetic dipole **m** in an external **B** field is:

$$\mathbf{F} = \nabla(\mathbf{m}\cdot\mathbf{B})$$

This implies that energy associated with aligning a magnetic dipole **m** in an external **B** field is given by:

$$U = -\mathbf{m}\cdot\mathbf{B}$$

Macroscopic energies --

It can be shown that: $$W_B = \frac{1}{2}\int d^3r\, \mathbf{B}(\mathbf{r})\cdot\mathbf{H}(\mathbf{r})$$

In analogy to: $$W_E = \frac{1}{2}\int d^3r\, \mathbf{E}(\mathbf{r})\cdot\mathbf{D}(\mathbf{r})$$

Full electrodynamics with time varying fields and sources

Maxwell's equations

Image of statue
in Edinburgh

JAMES Clerk-Maxwell was "the man who changed everything". He stands between Newton and Einstein in the triad of great scientists who shaped the modern world.

Duncan Macmillan -- 2008

http://www.clerkmaxwellfoundation.org/

Maxwell's equations

Coulomb's law: $\nabla \cdot \mathbf{D} = \rho_{free}$

Ampere-Maxwell's law: $\nabla \times \mathbf{H} - \frac{\partial \mathbf{D}}{\partial t} = \mathbf{J}_{free}$

Faraday's law: $\nabla \times \mathbf{E} + \frac{\partial \mathbf{B}}{\partial t} = 0$

No magnetic monopoles: $\nabla \cdot \mathbf{B} = 0$

Maxwell's equations

Microscopic or vacuum form $(\mathbf{P}=0;\ \mathbf{M}=0)$:

Coulomb's law: $\nabla \cdot \mathbf{E} = \rho / \varepsilon_0$

Ampere-Maxwell's law: $\nabla \times \mathbf{B} - \frac{1}{c^2}\frac{\partial \mathbf{E}}{\partial t} = \mu_0 \mathbf{J}$

Faraday's law: $\nabla \times \mathbf{E} + \frac{\partial \mathbf{B}}{\partial t} = 0$

No magnetic monopoles: $\nabla \cdot \mathbf{B} = 0$

$$\Rightarrow c^2 = \frac{1}{\varepsilon_0 \mu_0}$$

Formulation of Maxwell's equations in terms of vector and scalar potentials

$$\nabla \cdot \mathbf{B} = 0 \qquad \Rightarrow \; \mathbf{B} = \nabla \times \mathbf{A}$$

$$\nabla \times \mathbf{E} + \frac{\partial \mathbf{B}}{\partial t} = 0 \quad \Rightarrow \nabla \times \left(\mathbf{E} + \frac{\partial \mathbf{A}}{\partial t} \right) = 0$$

$$\mathbf{E} + \frac{\partial \mathbf{A}}{\partial t} = -\nabla \Phi$$

$$\text{or} \quad \mathbf{E} = -\nabla \Phi - \frac{\partial \mathbf{A}}{\partial t}$$

Formulation of Maxwell's equations in terms of vector and scalar potentials -- continued

$$\nabla \cdot \mathbf{E} = \rho / \varepsilon_0 :$$

$$-\nabla^2 \Phi - \frac{\partial \left(\nabla \cdot \mathbf{A} \right)}{\partial t} = \rho / \varepsilon_0$$

$$\nabla \times \mathbf{B} - \frac{1}{c^2} \frac{\partial \mathbf{E}}{\partial t} = \mu_0 \mathbf{J}$$

$$\nabla \times \left(\nabla \times \mathbf{A} \right) + \frac{1}{c^2} \left(\frac{\partial \left(\nabla \Phi \right)}{\partial t} + \frac{\partial^2 \mathbf{A}}{\partial t^2} \right) = \mu_0 \mathbf{J}$$

Formulation of Maxwell's equations in terms of vector and scalar potentials -- continued

Analysis of the scalar and vector potential equations:

$$-\nabla^2\Phi - \frac{\partial(\nabla\cdot\mathbf{A})}{\partial t} = \rho/\varepsilon_0$$

$$\nabla\times(\nabla\times\mathbf{A}) + \frac{1}{c^2}\left(\frac{\partial(\nabla\Phi)}{\partial t} + \frac{\partial^2\mathbf{A}}{\partial t^2}\right) = \mu_0\mathbf{J}$$

Coulomb gauge form -- require $\nabla\cdot\mathbf{A}_C = 0$

$$-\nabla^2\Phi_C = \rho/\varepsilon_0$$

$$-\nabla^2\mathbf{A}_C + \frac{1}{c^2}\frac{\partial^2\mathbf{A}_C}{\partial t^2} + \frac{1}{c^2}\frac{\partial(\nabla\Phi_C)}{\partial t} = \mu_0\mathbf{J}$$

Note that $\mathbf{J} = \mathbf{J}_l + \mathbf{J}_t$ with $\nabla\times\mathbf{J}_l = 0$ and $\nabla\cdot\mathbf{J}_t = 0$

Formulation of Maxwell's equations in terms of vector and scalar potentials -- continued

Coulomb gauge form - - require $\nabla \cdot \mathbf{A}_C = 0$

$$-\nabla^2 \Phi_C = \rho / \varepsilon_0$$

$$-\nabla^2 \mathbf{A}_C + \frac{1}{c^2}\frac{\partial^2 \mathbf{A}_C}{\partial t^2} + \frac{1}{c^2}\frac{\partial(\nabla \Phi_C)}{\partial t} = \mu_0 \mathbf{J}$$

Note that $\mathbf{J} = \mathbf{J}_l + \mathbf{J}_t$ with $\nabla \times \mathbf{J}_l = 0$ and $\nabla \cdot \mathbf{J}_t = 0$

Continuity equation for charge and current density:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot \mathbf{J}_l = 0 \qquad \Rightarrow \frac{\partial \rho}{\partial t} = -\nabla \cdot \mathbf{J}_l = -\varepsilon_0 \nabla \cdot \frac{\partial(\nabla \Phi_C)}{\partial t}$$

$$\Rightarrow \frac{1}{c^2}\frac{\partial(\nabla \Phi_C)}{\partial t} = \varepsilon_0 \mu_0 \frac{\partial(\nabla \Phi_C)}{\partial t} = \mu_0 \mathbf{J}_l$$

$$-\nabla^2 \mathbf{A}_C + \frac{1}{c^2}\frac{\partial^2 \mathbf{A}_C}{\partial t^2} = \mu_0 \mathbf{J}_t$$

Formulation of Maxwell's equations in terms of vector and scalar potentials -- continued

Analysis of the scalar and vector potential equations:

$$-\nabla^2\Phi - \frac{\partial(\nabla\cdot\mathbf{A})}{\partial t} = \rho/\varepsilon_0$$

$$\nabla\times(\nabla\times\mathbf{A}) + \frac{1}{c^2}\left(\frac{\partial(\nabla\Phi)}{\partial t} + \frac{\partial^2\mathbf{A}}{\partial t^2}\right) = \mu_0\mathbf{J}$$

Lorentz gauge form -- require $\nabla\cdot\mathbf{A}_L + \frac{1}{c^2}\frac{\partial\Phi_L}{\partial t} = 0$

$$-\nabla^2\Phi_L + \frac{1}{c^2}\frac{\partial^2\Phi_L}{\partial t^2} = \rho/\varepsilon_0$$

$$-\nabla^2\mathbf{A}_L + \frac{1}{c^2}\frac{\partial^2\mathbf{A}_L}{\partial t^2} = \mu_0\mathbf{J}$$

Formulation of Maxwell's equations in terms of vector and scalar potentials -- continued

$$\text{Lorentz gauge form -- require } \nabla \cdot \mathbf{A}_L + \frac{1}{c^2}\frac{\partial \Phi_L}{\partial t} = 0$$

$$-\nabla^2 \Phi_L + \frac{1}{c^2}\frac{\partial^2 \Phi_L}{\partial t^2} = \rho / \varepsilon_0$$

$$-\nabla^2 \mathbf{A}_L + \frac{1}{c^2}\frac{\partial^2 \mathbf{A}_L}{\partial t^2} = \mu_0 \mathbf{J}$$

$$\text{Alternate potentials:} \quad \mathbf{A}'_L = \mathbf{A}_L + \nabla\Lambda \quad \text{and} \quad \Phi'_L = \Phi_L - \frac{\partial \Lambda}{\partial t}$$

$$\text{Yields same physics provided that:} \quad \nabla^2\Lambda - \frac{1}{c^2}\frac{\partial^2 \Lambda}{\partial t^2} = 0$$