PHY 712 Electrodynamics
10-10:50 AM MWF in Olin 103

Class notes for Lecture 13:

Continue reading Chap. 5 – Sec. 5.6-5.7 in JDJ

A. Examples of magnetostatic fields

B. Magnetic dipoles

C. Hyperfine interaction

$$\mathcal{H}_{HF} = \frac{\mu_0}{4\pi}\left(\frac{3(\boldsymbol{\mu}_N \cdot \hat{\mathbf{r}})(\boldsymbol{\mu}_e \cdot \hat{\mathbf{r}}) - \boldsymbol{\mu}_N \cdot \boldsymbol{\mu}_e}{r^3} + \frac{8\pi}{3}\boldsymbol{\mu}_N \cdot \boldsymbol{\mu}_e \delta(\mathbf{r}) + \frac{e}{m_e}\left\langle \frac{\mathbf{L} \cdot \boldsymbol{\mu}_N}{r^3} \right\rangle \right)$$

Physics Colloquium

- Thursday -

February 13, 2025

Uncovering histone epigenetic biology through de novo protein design

The hierarchical systems of epigenetics, particularly chromatin architecture, regulate DNA-templated processes. Histone post-translational modifications maintain cell homeostasis. The specific PTM response is governed by cooperative interactions between multiple binding partners. Linking histone PTMs to elicited biological responses is challenging. Quantitative and orthogonal experiments within the nucleosome interactome are needed to understand the chemical and biophysical basis of PTMs influencing dynamic epigenetic states. We aim to develop novel de novo proteins as orthogonal tools for in vitro and cellular mechanism probing. Our de novo scaffolds selectively bind histone PTMs and disease-associated mutations and harness the ability to turn off and on protein-protein interactions under exogenous control. This represents a significant advancement in deconvolving transient and cooperative interactions underpinning chromatin regulation and epigenetic states. These tools and methodologies can be applied to other research questions, providing a framework for investigating other complex biological systems.

Professor Katherine Albanese
Department of Chemistry
Wake Forest University

Reception 3:30
Olin Lobby

Colloquium 4:00
Olin 101

Course schedule for Spring 2025

(Preliminary schedule -- subject to frequent adjustment.)

	Lecture date	JDJ Reading	Topic	HW	Due date
1	Mon: 01/13/2025	Chap. 1 & Appen.	Introduction, units and Poisson equation	#1	01/15/2025
2	Wed: 01/15/2025	Chap. 1	Electrostatic energy calculations	#2	01/17/2025
3	Fri: 01/17/2025	Chap. 1	Electrostatic energy calculations	#3	01/22/2025
	Mon: 01/20/2025	No Class	Martin Luther King Jr. Holiday		
4	Wed: 01/22/2025	Chap. 1	Electrostatic potentials and fields	#4	01/24/2025
5	Fri: 01/24/2025	Chap. 1 - 3	Poisson's equation in multiple dimensions		
6	Mon: 01/27/2025	Chap. 1 - 3	Brief introduction to numerical methods	#5	01/29/2025
7	Wed: 01/29/2025	Chap. 2 & 3	Image charge constructions	#6	01/31/2025
8	Fri: 01/31/2025	Chap. 2 & 3	Poisson equation in cylindrical geometries	#7	02/03/2025
9	Mon: 02/03/2025	Chap. 3 & 4	Spherical geometry and multipole moments	#8	02/05/2025
10	Wed: 02/05/2025	Chap. 4	Dipoles and Dielectrics	#9	02/07/2025
11	Fri: 02/07/2025	Chap. 4	Dipoles and Dielectrics	#10	02/10/2025
12	Mon: 02/10/2025	Chap. 5	Magnetostatics	#11	02/12/2025
13	Wed: 02/12/2025	Chap. 5	Magnetic dipoles and hyperfine interactions	#12	02/14/2025
14	Fri: 02/14/2025	Chap. 5	Magnetic materials and boundary value problems		
15	Mon: 02/17/2025	Chap. 6	Maxwell's Equations		

PHY 712 – Problem Set #12

Assigned: 02/12/2025 Due: 02/14/2025

Continue reading Chapter 5 in **Jackson** and the detailed lecturenotes for Lecture 13.

1. One of the identities used to derive the hyperfine interaction expression given in the detailed lecture notes is

$$\int d\Omega \frac{\hat{\mathbf{r}}}{|\mathbf{r}-\mathbf{r}'|} = \frac{4\pi}{3}\frac{r_<}{r_>^2}\hat{\mathbf{r}}'.$$

Here, $\mathbf{r}'$ is a fixed radial vector, $d\Omega \equiv \sin\theta d\theta d\varphi$, the integral is taken over $0 \leq \varphi \leq 2\pi$ and $0 \leq \theta \leq \pi$, and

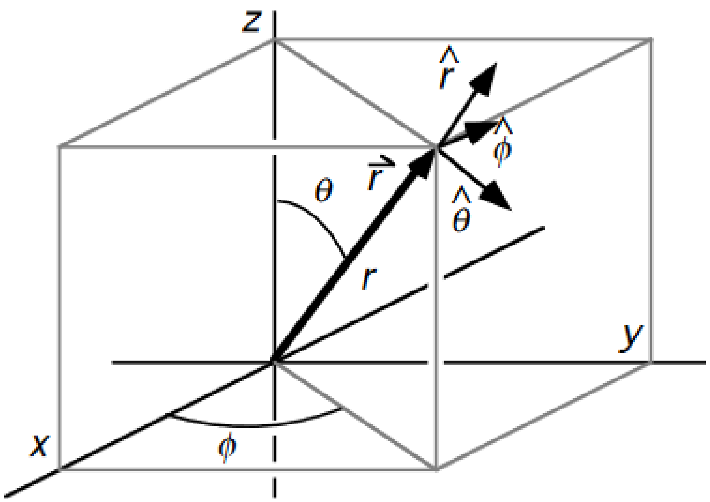
$$\hat{\mathbf{r}} \equiv \frac{\mathbf{r}}{r} = \sin\theta\cos\varphi\hat{\mathbf{x}} + \sin\theta\sin\varphi\hat{\mathbf{y}} + \cos\theta\hat{\mathbf{z}}.$$

Verify the identity.

Comment about spherical polar coordinates

Ref: https://www.cpp.edu/~ajm/materials/delsph.pdf

Spherical Coordinates



Transforms

The forward and reverse coordinate transformations are

$$r = \sqrt{x^2 + y^2 + z^2}$$

$$\theta = \arctan\left(\sqrt{x^2 + y^2}, z\right)$$

$$\phi = \arctan(y, x)$$

$$x = r\sin\theta\cos\phi$$

$$y = r\sin\theta\sin\phi$$

$$z = r\cos\theta$$

where we *formally* take advantage of the *two argument* arctan function to eliminate quadrant confusion.

Unit Vectors

The unit vectors in the spherical coordinate system are functions of position. It is convenient to express them in terms of the *spherical* coordinates and the unit vectors of the *rectangular* coordinate system which are *not* themselves functions of position.

$$\hat{r} = \frac{\vec{r}}{r} = \frac{x\hat{x} + y\hat{y} + z\hat{z}}{r} = \hat{x}\sin\theta\cos\phi + \hat{y}\sin\theta\sin\phi + \hat{z}\cos\theta$$

$$\hat{\phi} = \frac{\hat{z}\times\hat{r}}{\sin\theta} = -\hat{x}\sin\phi + \hat{y}\cos\phi$$

$$\hat{\theta} = \hat{\phi}\times\hat{r} = \hat{x}\cos\theta\cos\phi + \hat{y}\cos\theta\sin\phi - \hat{z}\sin\theta$$

$$\hat{r} = \frac{\vec{r}}{r} = \frac{x\hat{x} + y\hat{y} + z\hat{z}}{r} = \hat{x}\sin\theta\cos\phi + \hat{y}\sin\theta\sin\phi + \hat{z}\cos\theta$$

$$\hat{\phi} = \frac{\hat{z}\times\hat{r}}{\sin\theta} = -\hat{x}\sin\phi + \hat{y}\cos\phi$$

$$\hat{\theta} = \hat{\phi}\times\hat{r} = \hat{x}\cos\theta\cos\phi + \hat{y}\cos\theta\sin\phi - \hat{z}\sin\theta$$

Note result given in "detailed" pdf file:

In order to evaluate the vector potential (1) for this problem, we can make use of the expansion:

$$\frac{1}{|\mathbf{r}-\mathbf{r}'|} = \sum_{lm} \frac{4\pi}{2l+1} \frac{r_<^l}{r_>^{l+1}} Y_{lm}(\hat{\mathbf{r}}) Y_{lm}^*(\hat{\mathbf{r}'}). \tag{3}$$

Noting that

$$\mathbf{r}' = r' \sqrt{\frac{4\pi}{3}} \left(Y_{1-1}(\hat{\mathbf{r}'}) \frac{\hat{\mathbf{x}} + \mathbf{i}\hat{\mathbf{y}}}{\sqrt{2}} + Y_{11}(\hat{\mathbf{r}'}) \frac{-\hat{\mathbf{x}} + \mathbf{i}\hat{\mathbf{y}}}{\sqrt{2}} + Y_{10}(\hat{\mathbf{r}'})\hat{\mathbf{z}} \right), \tag{4}$$

we see that the angular integral in Eq. (1) can be simplified with the use of the identity:

$$\int d\Omega' \sum_{lm} Y_{lm}(\hat{\mathbf{r}}) Y_{lm}^*(\hat{\mathbf{r}'})\ \mathbf{r}' = \frac{r'}{r}\mathbf{r} \ \equiv r'\ \hat{\mathbf{r}}\ . \tag{5}$$

https://users.wfu.edu/natalie/s25phy712/lecturenote/

Lecture Notes

- Lecture 1 -- Introduction and electrostatics PP slides PDF
- Lecture 2 -- Electrostatic energy calculations PP slides PDF
- Lecture 3 -- Electrostatic energy calculations PP slides PDF Ewaldnotes PDF Maple file for CsCl Maple PDF for CsCl
- Lecture 4 -- Solutions of the Poisson and Laplace equations with George Green's help PP slides PDF
- Lecture 5 -- Solution of Poisson and Lapace equations in multiple dimensions PP slides PDF
- Lecture 6 -- Brief introduction to numerical methods for solving electrostatic problems PP slides PDF Detailed PDF
- Lecture 7 -- Image charge methods PP slides PDF
- Lecture 8 -- Electrostatics in cylindrical coordinates PP slides PDF
- Lecture 9 -- Electrostatics in spherical coordinates PP slides PDF
- Lecture 10 -- Electrostatics and multipole moments PP slides PDF
- Lecture 11 -- Polarization and dielectric response PP slides PDF
- Lecture 12 -- Introduction to magnetostatics PP slides PDF
- Lecture 13 -- Magnetic dipoles and hyperfine interactions PP slides PDF Detailed PDF

Example macroscopic localized current source --

For the model current density --

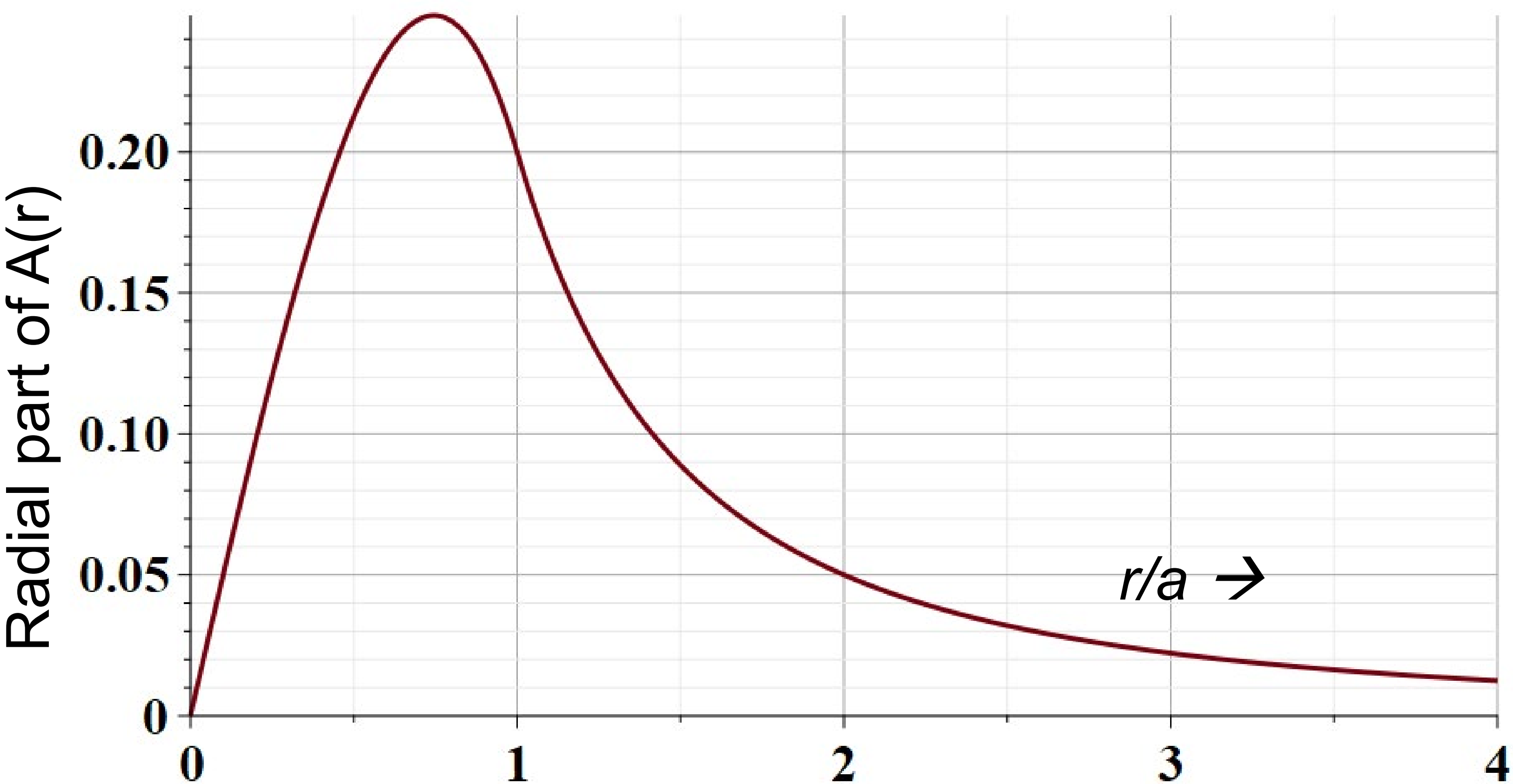
$$\mathbf{J}(\mathbf{r}) = \begin{cases} \rho_0 \boldsymbol{\omega} \times \mathbf{r} & \text{for r } \leq a \\ 0 & \text{otherwise} \end{cases}$$

Here ρ_0 is a charge density constant $\boldsymbol{\omega}$ is a constant angular velocity

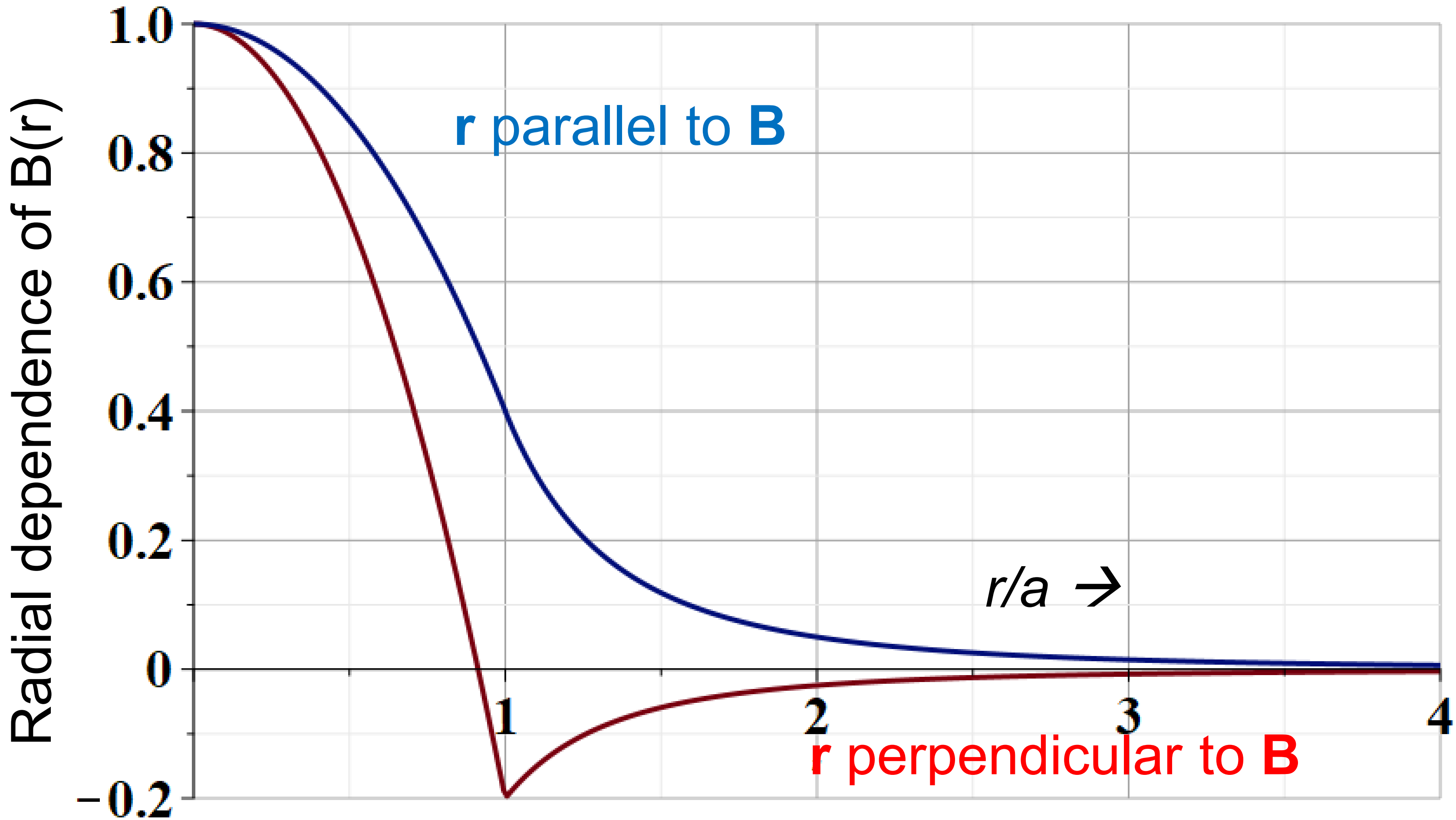
$$\mathbf{A}(\mathbf{r}) = \begin{cases} \frac{\mu_0 \rho_0}{3} \boldsymbol{\omega} \times \mathbf{r} \left(\frac{a^2}{2} - \frac{3r^2}{10} \right) & \text{for } r \leq a \\ \\ \frac{\mu_0 \rho_0}{3} \boldsymbol{\omega} \times \mathbf{r} \frac{a^5}{5r^3} & \text{for } r \geq a \end{cases} .$$

$$\mathbf{B}(\mathbf{r}) = \nabla \times \mathbf{A}(\mathbf{r}) = \begin{cases} \frac{\mu_0 \rho_0}{3} \left[\boldsymbol{\omega} \left(a^2 - \frac{6}{5} r^2 \right) + \frac{3}{5} \mathbf{r} (\boldsymbol{\omega} \cdot \mathbf{r}) \right] & \text{for } r \leq a \\ \frac{\mu_0 \rho_0}{3} \left[-\boldsymbol{\omega} \frac{a^5}{5r^3} + \frac{3a^5}{5r^5} \mathbf{r} (\boldsymbol{\omega} \cdot \mathbf{r}) \right] & \text{for } r \geq a \end{cases}$$

$$\mathbf{A}(\mathbf{r}) = \begin{cases} \frac{\mu_0\rho_0}{3}\boldsymbol{\omega}\times\mathbf{r}\left(\frac{a^2}{2}-\frac{3r^2}{10}\right) & \text{for } r \le a \\ \frac{\mu_0\rho_0}{3}\boldsymbol{\omega}\times\mathbf{r}\frac{a^5}{5r^3} & \text{for } r \ge a \end{cases}.$$



$$\mathbf{B}(\mathbf{r}) = \nabla \times \mathbf{A}(\mathbf{r}) = \begin{cases} \frac{\mu_0 \rho_0}{3} \left[\boldsymbol{\omega} \left(a^2 - \frac{6}{5} r^2 \right) + \frac{3}{5} \mathbf{r}(\boldsymbol{\omega} \cdot \mathbf{r}) \right] & \text{for } r \leq a \\ \frac{\mu_0 \rho_0}{3} \left[-\boldsymbol{\omega} \frac{a^5}{5r^3} + \frac{3a^5}{5r^5} \mathbf{r}(\boldsymbol{\omega} \cdot \mathbf{r}) \right] & \text{for } r \geq a \end{cases}$$



Various forms of Ampere's law :

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

$$\text{Vector potential:} \quad \mathbf{B}(\mathbf{r}) = \nabla \times \mathbf{A}(\mathbf{r})$$

$$\text{For Coulomb gauge:} \quad \nabla \cdot \mathbf{A}(\mathbf{r}) = 0$$

$$\Rightarrow \nabla^2 \mathbf{A}(\mathbf{r}) = -\mu_0 \mathbf{J}(\mathbf{r})$$

For confined current density :

$$\mathbf{A}(\mathbf{r}) = \frac{\mu_0}{4\pi} \int d^3 r' \frac{\mathbf{J}(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|}$$

Other examples of current density sources:

Quantum mechanical expression for current density

for a particle of mass m_e and charge e and of probability amplitude $\Psi(\mathbf{r})$:

$$\mathbf{J}(\mathbf{r}) = -\frac{e\hbar}{2m_e i}\left(\Psi^*(\mathbf{r})\nabla\Psi(\mathbf{r}) - \Psi(\mathbf{r})\nabla\Psi^*(\mathbf{r})\right)$$

For an electron in a spherical potential (such as in an atom):

$$\Psi(\mathbf{r}) \equiv \Psi_{nlm_l}(\mathbf{r}) = R_{nl}(r)Y_{lm_l}(\hat{\mathbf{r}})$$

$$\mathbf{J}(\mathbf{r}) = \frac{e\hbar}{2m_e i}\left|R_{nl}(r)\right|^2 \frac{1}{r\sin\theta}\left(Y_{lm_l}{}^*(\hat{\mathbf{r}})\frac{\partial Y_{lm_l}(\hat{\mathbf{r}})}{\partial\varphi} - Y_{lm_l}(\hat{\mathbf{r}})\frac{\partial Y_{lm_l}{}^*(\hat{\mathbf{r}})}{\partial\varphi}\right)\hat{\boldsymbol{\varphi}}$$

$$= \frac{e\hbar}{m_e}\frac{m_l}{r\sin\theta}\left|\Psi_{nlm_l}(\mathbf{r})^2\right|\hat{\boldsymbol{\varphi}}$$

Note that: $\hat{\boldsymbol{\varphi}} = -\sin\varphi\hat{\mathbf{x}} + \cos\varphi\hat{\mathbf{y}} = \dfrac{\hat{\mathbf{z}}\times\mathbf{r}}{r\sin\theta}$

$$\mathbf{J}(\mathbf{r}) = \frac{e\hbar}{m_e}\frac{m_l}{r^2\sin^2\theta}\left|\Psi_{nlm_l}(\mathbf{r})\right|^2(\hat{\mathbf{z}}\times\mathbf{r})$$

Details of the electron orbital magnetic dipole moment

$$\mathbf{J}(\mathbf{r}) = \frac{e\hbar}{m_e}\frac{m_l}{r\sin\theta}\left|\Psi_{nlm_l}(\mathbf{r})^2\right|\hat{\boldsymbol{\varphi}}$$

Note that: $\hat{\boldsymbol{\varphi}} = -\sin\varphi\,\hat{\mathbf{x}} + \cos\varphi\,\hat{\mathbf{y}}$

Magnetic dipole moment:

$$\mathbf{m} = \frac{1}{2}\int d^3r'\,\mathbf{r}' \times \mathbf{J}(\mathbf{r}') = -\frac{e\hbar m_l}{2m_e}\int d^3r'\,\frac{\mathbf{r}' \times \hat{\boldsymbol{\varphi}}'}{r'\sin\theta'}\left|\Psi_{nlm_l}(\mathbf{r})^2\right|$$

$$= -\frac{e\hbar m_l}{2m_e}\int d^3r'\,\frac{-r'\hat{\boldsymbol{\theta}}'}{r'\sin\theta'}\left|\Psi_{nlm_l}(\mathbf{r})^2\right|$$

Note that: $\hat{\boldsymbol{\theta}} = \cos\theta\cos\varphi\,\hat{\mathbf{x}} + \cos\theta\sin\varphi\,\hat{\mathbf{y}} - \sin\theta\,\hat{\mathbf{z}}$

$$\mathbf{m} = -\frac{e\hbar m_l\hat{\mathbf{z}}}{2m_e}\int d^3r'\left|\Psi_{nlm_l}(\mathbf{r})^2\right|$$

$$= -\frac{e\hbar m_l}{2m_e}\hat{\mathbf{z}}$$

Note that $\frac{e\hbar}{2m_e}$ = "Bohr magneton"=9.274 010 0657 x 10^{-24} Joules/Tesla

Significance of magnetic dipole – multipole approximation to vector potential and magnetic field

Magnetic dipolar field

The magnetic dipole moment is defined by

$$\mathbf{m} = \frac{1}{2}\int d^3r'\mathbf{r}' \times \mathbf{J}(\mathbf{r}'),$$

with the corresponding potential

$$\mathbf{A}(\mathbf{r}) = \frac{\mu_0}{4\pi}\frac{\mathbf{m}\times\hat{\mathbf{r}}}{r^2},$$

and magnetostatic field

$$\mathbf{B}_{\mathbf{m}}(\mathbf{r}) = \frac{\mu_0}{4\pi}\left\{\frac{3\hat{\mathbf{r}}(\mathbf{m}\cdot\hat{\mathbf{r}}) - \mathbf{m}}{r^3} + \frac{8\pi}{3}\mathbf{m}\delta^3(\mathbf{r})\right\}.$$

Note that the electron orbital magnetic dipole moment, discussed in previous slides, is only one example of magnetic dipoles found in nature.

Many particles – electrons, protons, neutrons, composite nuclei, … have "intrinsic" magnetic dipole moments. For these, we may not be able to calculate the magnetic dipole moment from the formula

$$\mathbf{m} = \frac{1}{2}\int d^3r' \, \mathbf{r}' \times \mathbf{J}(\mathbf{r}')$$

but their moments can be measured, and they effect the fields and energies of the systems which contain them.

Summary of magnetic field generated by point magnetic dipole moment discussed in the detailed notes:

$$\mathbf{B}_{\boldsymbol{\mu}_e}(\mathbf{r}) = \frac{\mu_0}{4\pi}\left(\frac{3\hat{\mathbf{r}}\left(\boldsymbol{\mu}_e\cdot\hat{\mathbf{r}}\right)-\boldsymbol{\mu}_e}{r^3}+\frac{8\pi}{3}\boldsymbol{\mu}_e\delta(\mathbf{r})\right)$$

Magnetic field near nucleus due to orbiting electron:

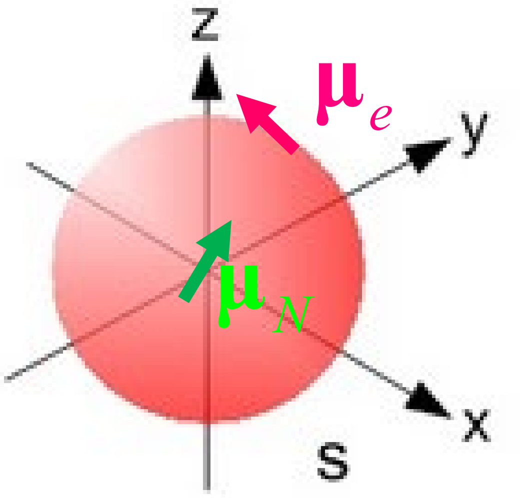
$$\mathbf{B}_O(\mathbf{r}) = \frac{\mu_0}{4\pi}\frac{e}{m_e}L_z\hat{\mathbf{z}}\left\langle\frac{1}{r^3}\right\rangle$$

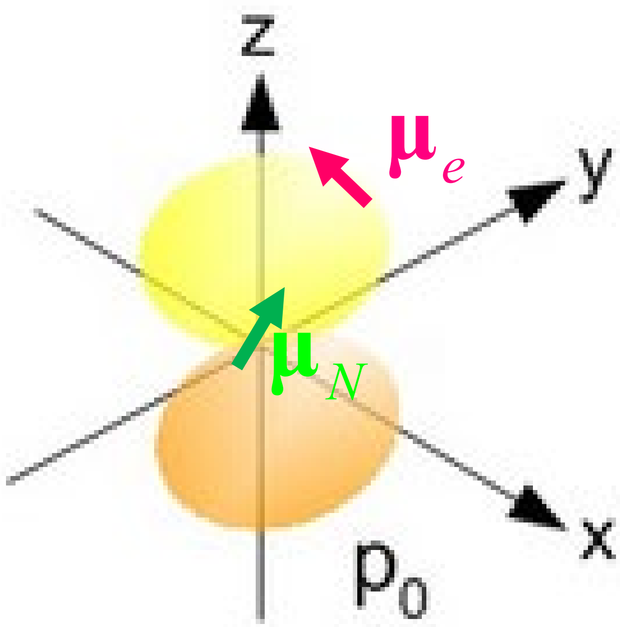
"Hyperfine" interaction energy:

$$\mathcal{H}_{HF} = -\boldsymbol{\mu}_N\cdot\left(\mathbf{B}_{\boldsymbol{\mu}_e}(\mathbf{r})+\mathbf{B}_O(\mathbf{r})\right)$$

$$= \frac{\mu_0}{4\pi}\left(\frac{3\left(\boldsymbol{\mu}_N\cdot\hat{\mathbf{r}}\right)\left(\boldsymbol{\mu}_e\cdot\hat{\mathbf{r}}\right)-\boldsymbol{\mu}_N\cdot\boldsymbol{\mu}_e}{r^3}+\frac{8\pi}{3}\boldsymbol{\mu}_N\cdot\boldsymbol{\mu}_e\delta(\mathbf{r})+\frac{e}{m_e}\left\langle\frac{\mathbf{L}\cdot\boldsymbol{\mu}_N}{r^3}\right\rangle\right)$$

$$\mathcal{H}_{HF} = \frac{\mu_0}{4\pi}\left(\frac{3(\boldsymbol{\mu}_N \cdot \hat{\mathbf{r}})(\boldsymbol{\mu}_e \cdot \hat{\mathbf{r}}) - \boldsymbol{\mu}_N \cdot \boldsymbol{\mu}_e}{r^3} + \frac{8\pi}{3}\boldsymbol{\mu}_N \cdot \boldsymbol{\mu}_e \delta(\mathbf{r}) + \frac{e}{m_e}\left\langle \frac{\mathbf{L} \cdot \boldsymbol{\mu}_N}{r^3} \right\rangle \right)$$





Here, $\boldsymbol{\mu}_e$ $\Rightarrow$ Intrinsic electron magnetic dipole moment

$\boldsymbol{\mu}_N$ $\Rightarrow$ Intrinsic nuclear magnetic dipole moment

$\frac{e\mathbf{L}}{m_e}$ $\Rightarrow$ Electron orbital mgnetic dipole moment (**L** denotes orbital momentum operator)