

Anapole Moment Calculated within Nuclear DFT

Herlik Wibowo

Collaborators: B. C. Backes, M. Kanerva, J. Dobaczewski,
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1

Anapole Moment and Fundamental Symmetry

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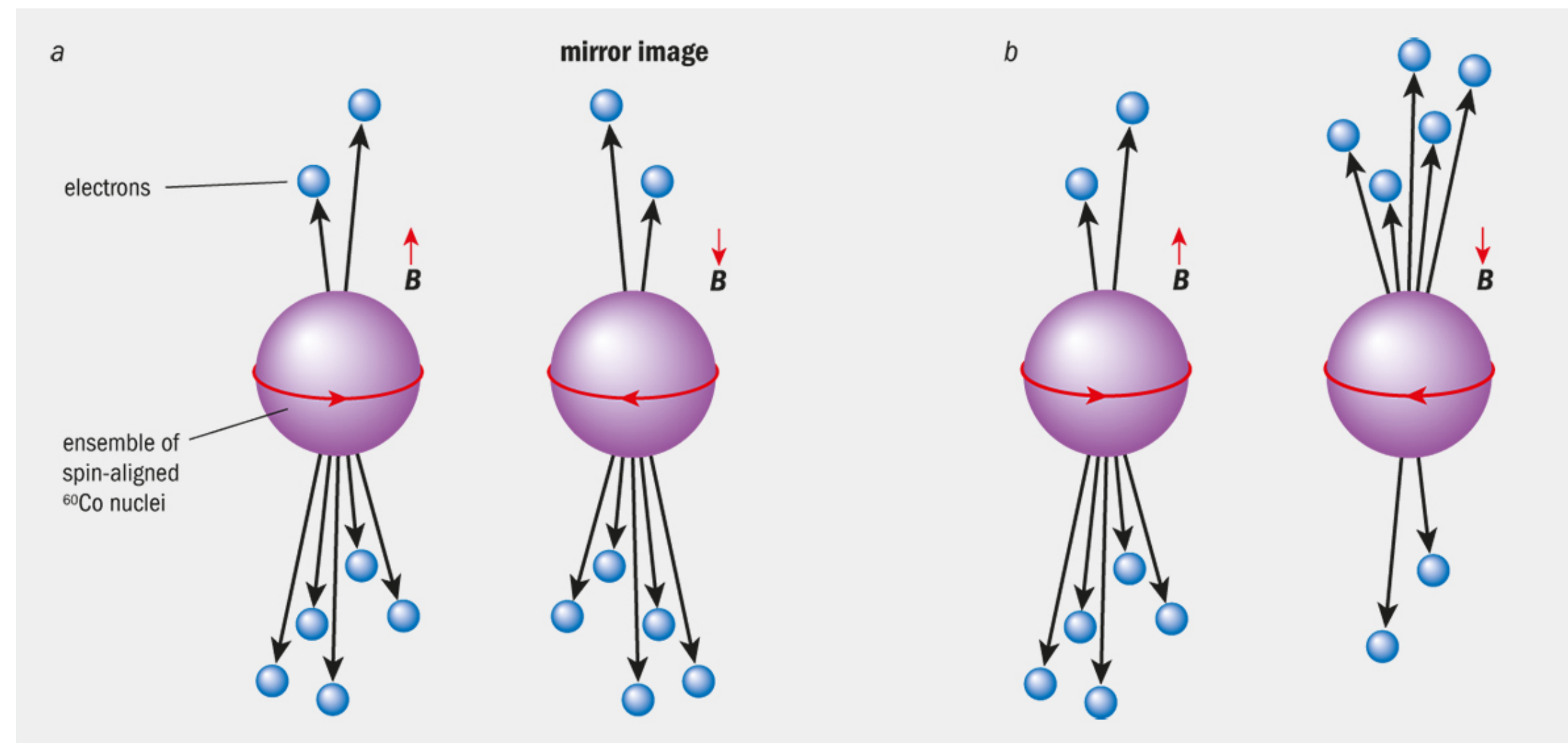
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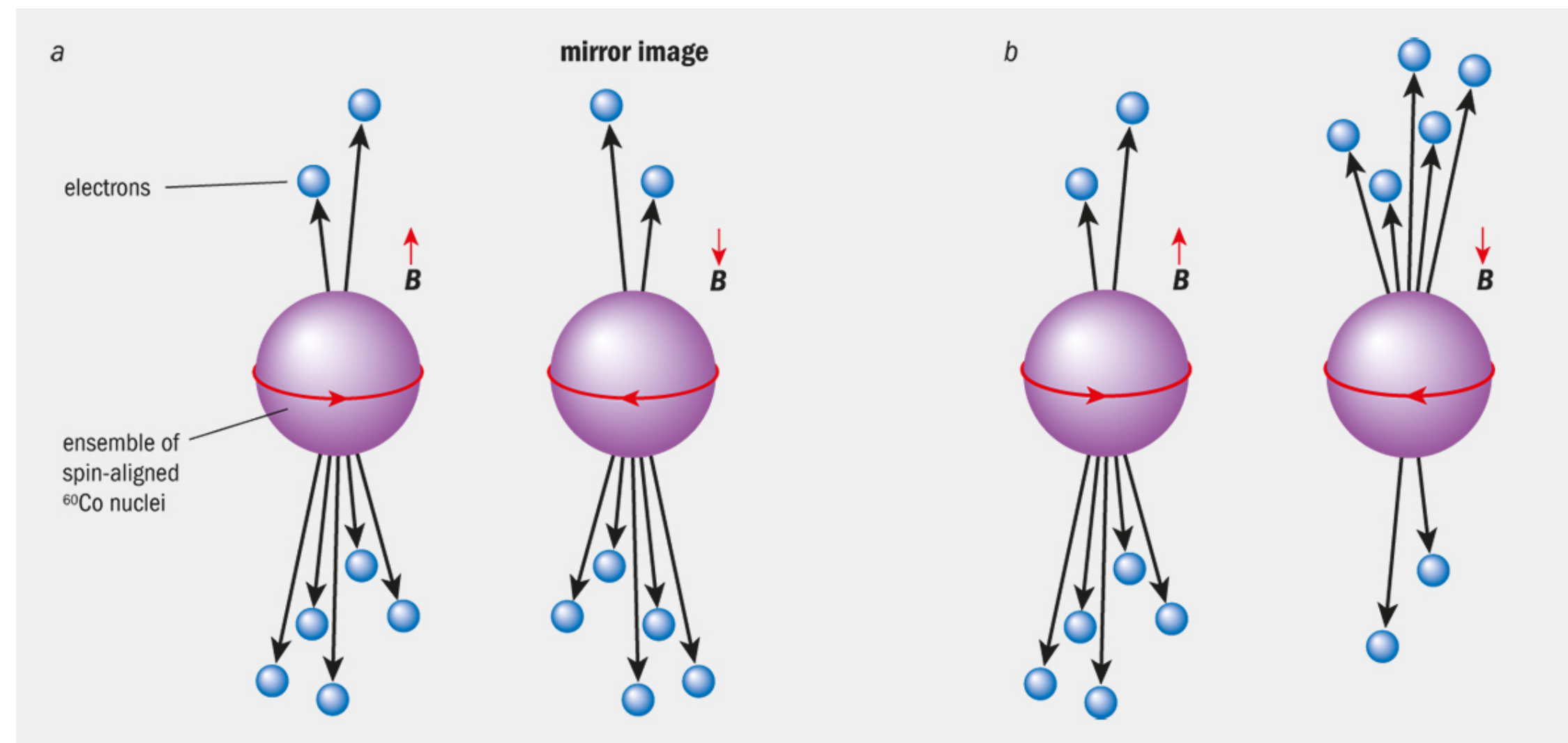
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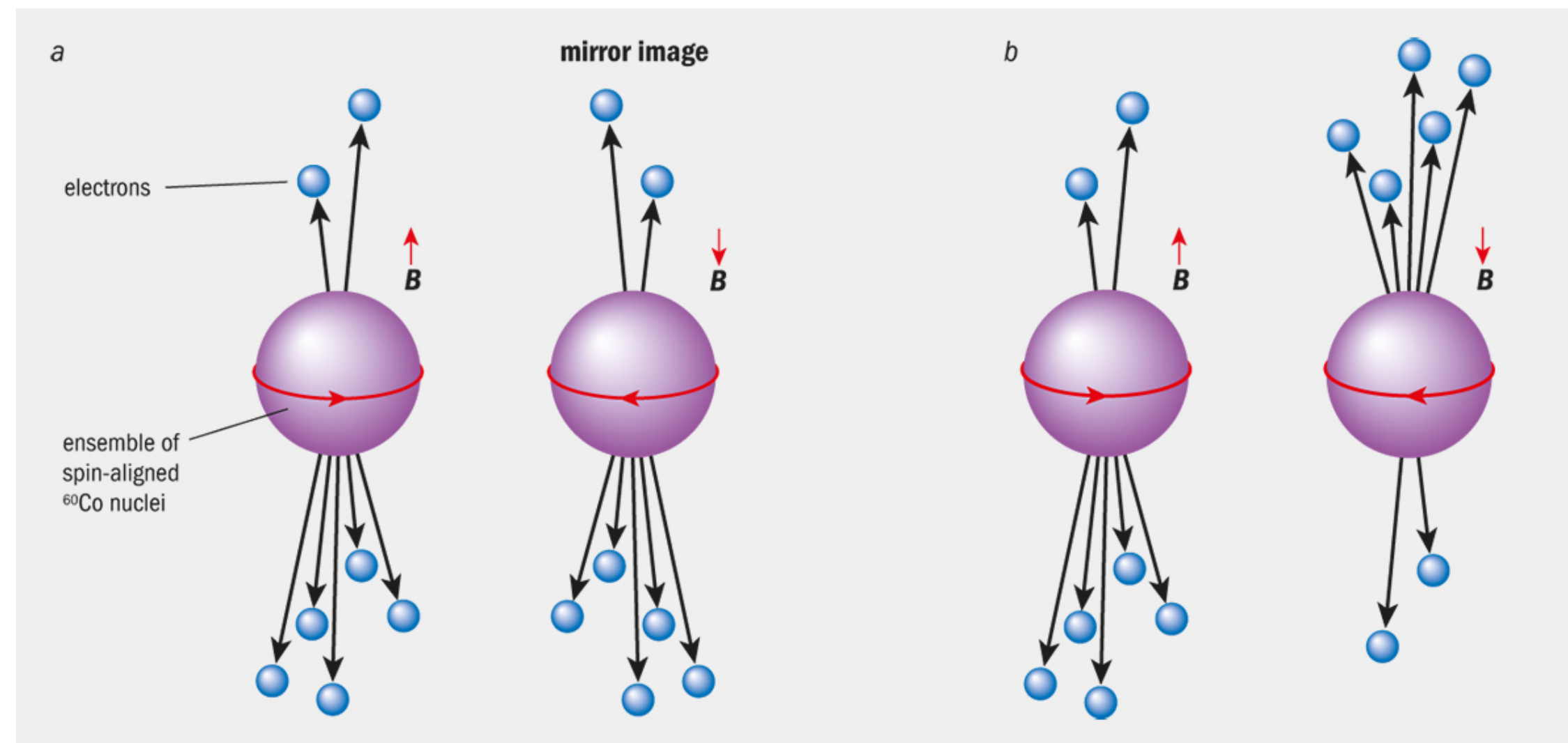


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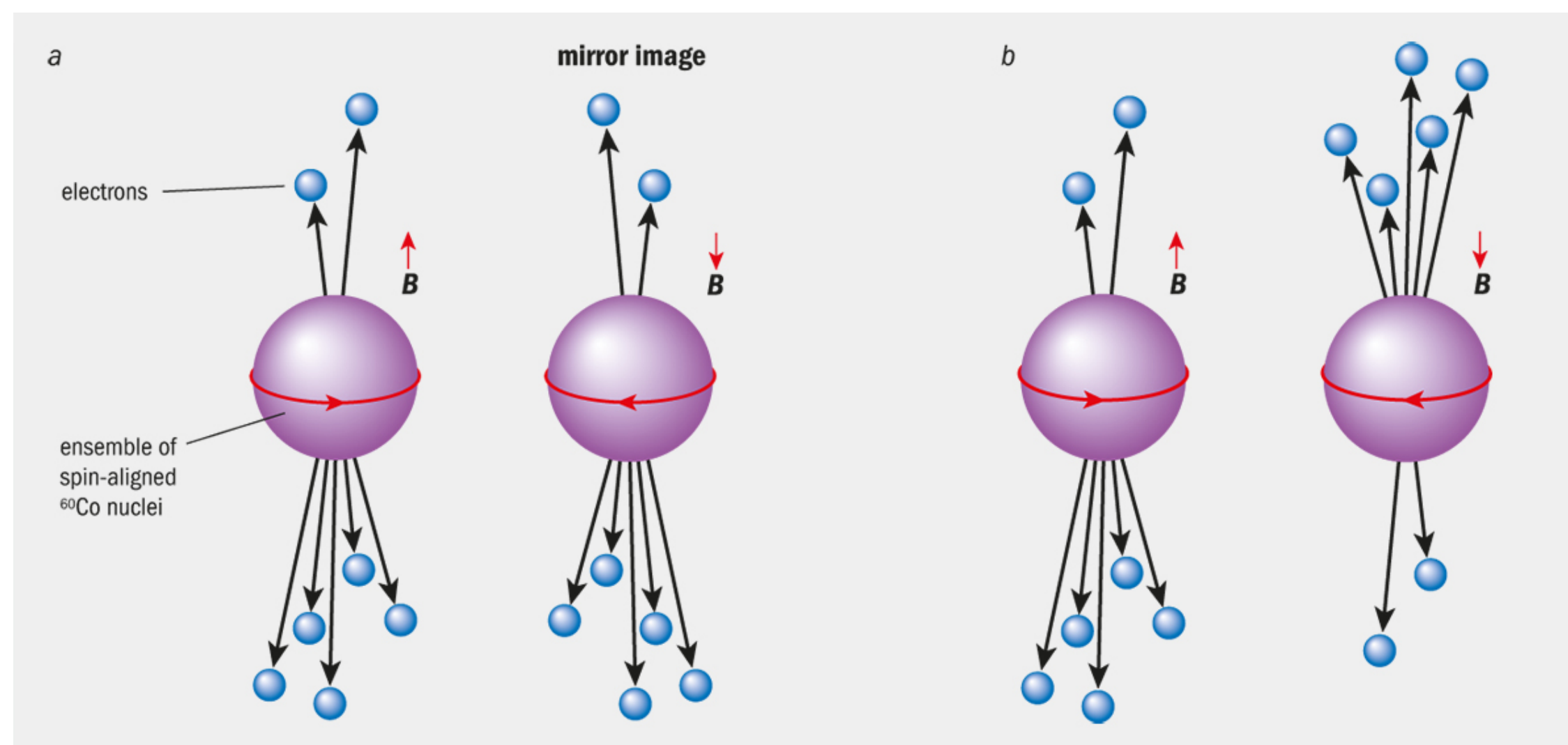


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- ★ In 1997, C. S. Wood and collaborators experimentally discovered the anapole moment in cesium-133 [C. S. Wood, et al., *Science* **275**, 1759 (1997)].

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Anapole Moment in Classical Electromagnetism

A. Zangwill, *Modern Electrodynamics*

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The multipole expansion of the vector potential $\mathbf{A}(\mathbf{r})$ in the Cartesian coordinates reads

$$\begin{aligned}
 A_k(\mathbf{r}) &= \frac{\mu_0}{4\pi} \left\{ \left[\int d^3s \, j_k(\mathbf{s}) \right] \frac{1}{r} - \left[\frac{1}{1!} \int d^3s \, j_k(\mathbf{s}) s_\ell \right] \nabla_\ell \frac{1}{r} + \left[\frac{1}{2!} \int d^3s \, j_k(\mathbf{s}) s_\ell s_m \right] \nabla_\ell \nabla_m \frac{1}{r} - \dots \right\} \\
 &\equiv \frac{\mu_0}{4\pi} \sum_{n=1}^{\infty} (-1)^n T_{k\ell\dots m}^{(n)} \underbrace{\nabla_\ell \dots \nabla_m}_{n \text{ terms}} \frac{1}{r}.
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Here tensor $T_{k\ell\dots m}^{(n)}$ is defined as

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Anapole moment is a part of magnetic quadrupole tensor, $T_{k\ell m}^{(2)}$.

$$T_{k\ell m}^{(2)} = \frac{1}{2} \int d^3s j_k(\mathbf{s}) s_\ell s_m = \frac{1}{3} \epsilon_{kil} \int d^3s (\mathbf{s} \times \mathbf{j})_i s_m \equiv \frac{1}{3} \epsilon_{kil} \int d^3s N_i s_m.$$

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Anapole Moment in Classical Electromagnetism

Anapole Moment in Classical Electromagnetism

Let us now decompose the product $N_i s_m$ into

$$N_i s_m = \frac{1}{2}(N_i s_m + N_m s_i) + \frac{1}{2}(N_i s_m - N_m s_i).$$

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The antisymmetric term gives us the anapole part, that is

$$T_{klm}^{(2;\text{anapole})} = \frac{1}{6} \epsilon_{kil} \int d^3 s (N_i s_m - N_m s_i) = \frac{1}{4\pi} (\delta_{km} a_l - \delta_{lm} a_k),$$

where the anapole moment \mathbf{a} is defined as

$$\mathbf{a} = \frac{2}{3} \pi \int d^3 s [\mathbf{s}(\mathbf{s} \cdot \mathbf{j}) - s^2 \mathbf{j}].$$

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Steady-current condition: $\nabla_{\mathbf{s}} \cdot \mathbf{j} + \underbrace{\partial \rho / \partial t}_{=0} = 0 \rightarrow \nabla_{\mathbf{s}} \cdot \mathbf{j} = 0$



4

Anapole Moment in Classical Electromagnetism

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$$\mathbf{A}^{(\text{anapole})}(\mathbf{r}) = \mu_0 \left[\mathbf{a} \delta(\mathbf{r}) + \nabla(\mathbf{a} \cdot \nabla) \frac{1}{4\pi r} \right].$$

The magnetic field $\mathbf{B}^{(\text{anapole})} = \nabla \times \mathbf{A}^{(\text{anapole})}$ reads

$$\mathbf{B}^{(\text{anapole})}(\mathbf{r}) = -\mu_0 \mathbf{a} \times \nabla \delta(\mathbf{r}),$$

since $\nabla \times \nabla f(\mathbf{r}) = 0$.

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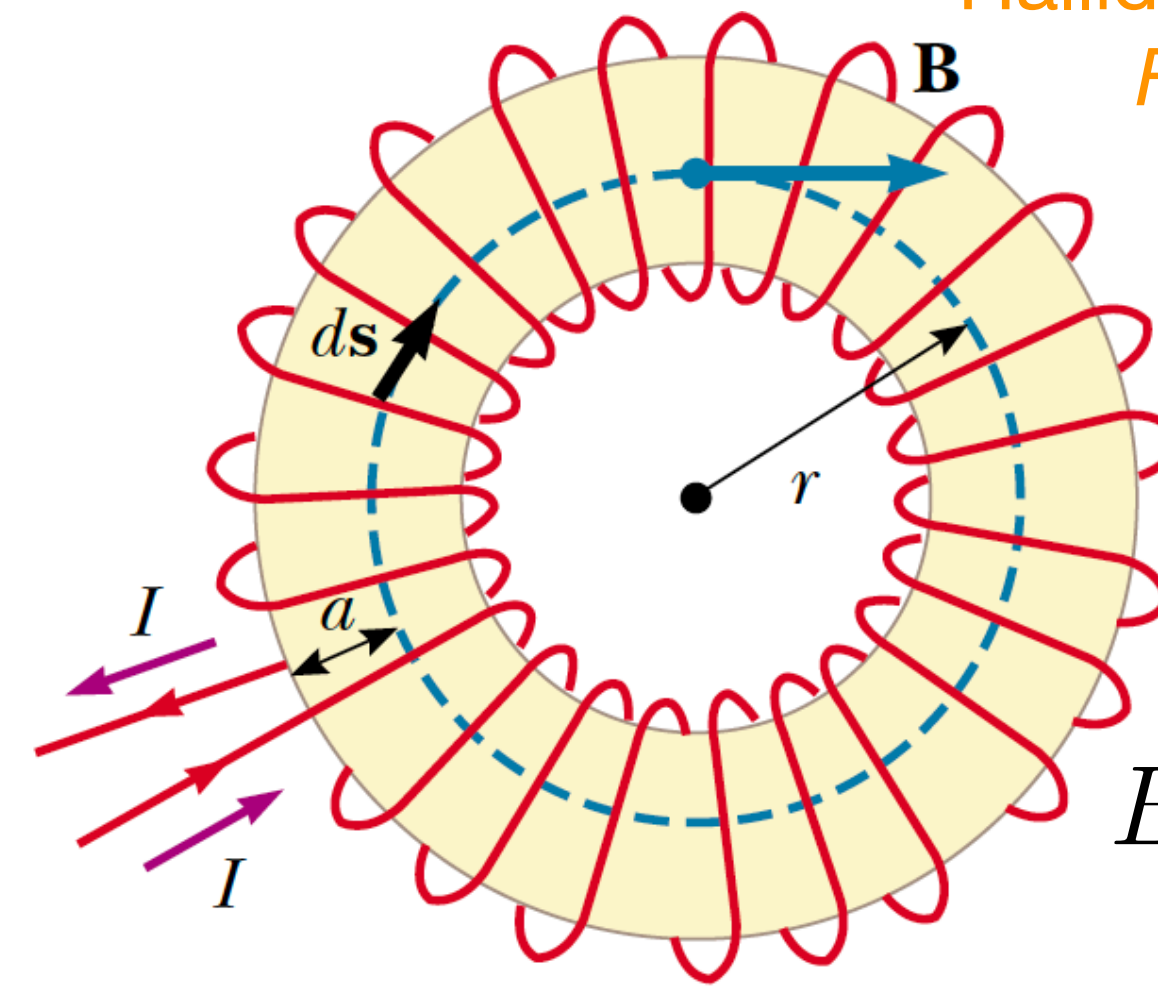
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Halliday, Resnick, and Walker,
Fundamentals of Physics



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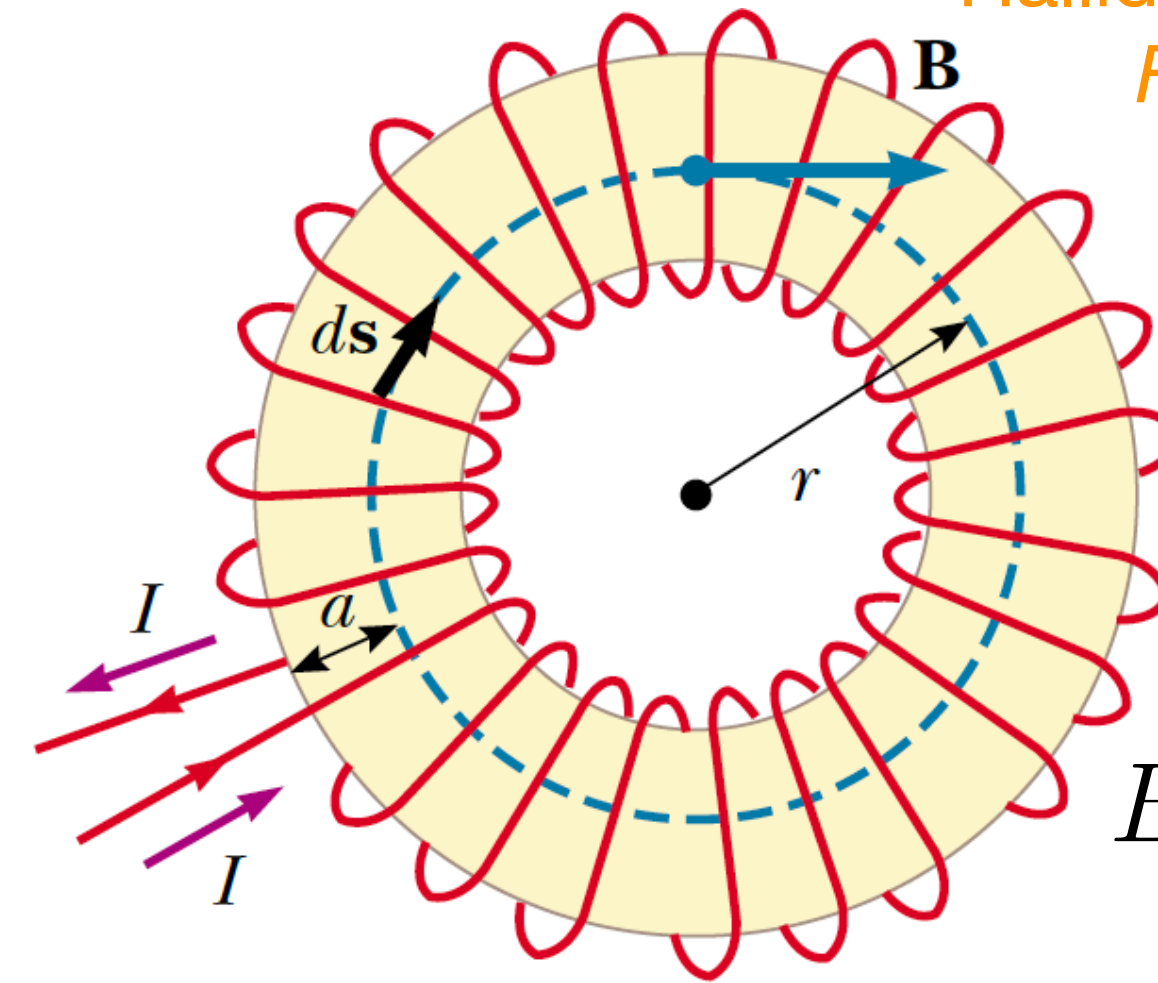
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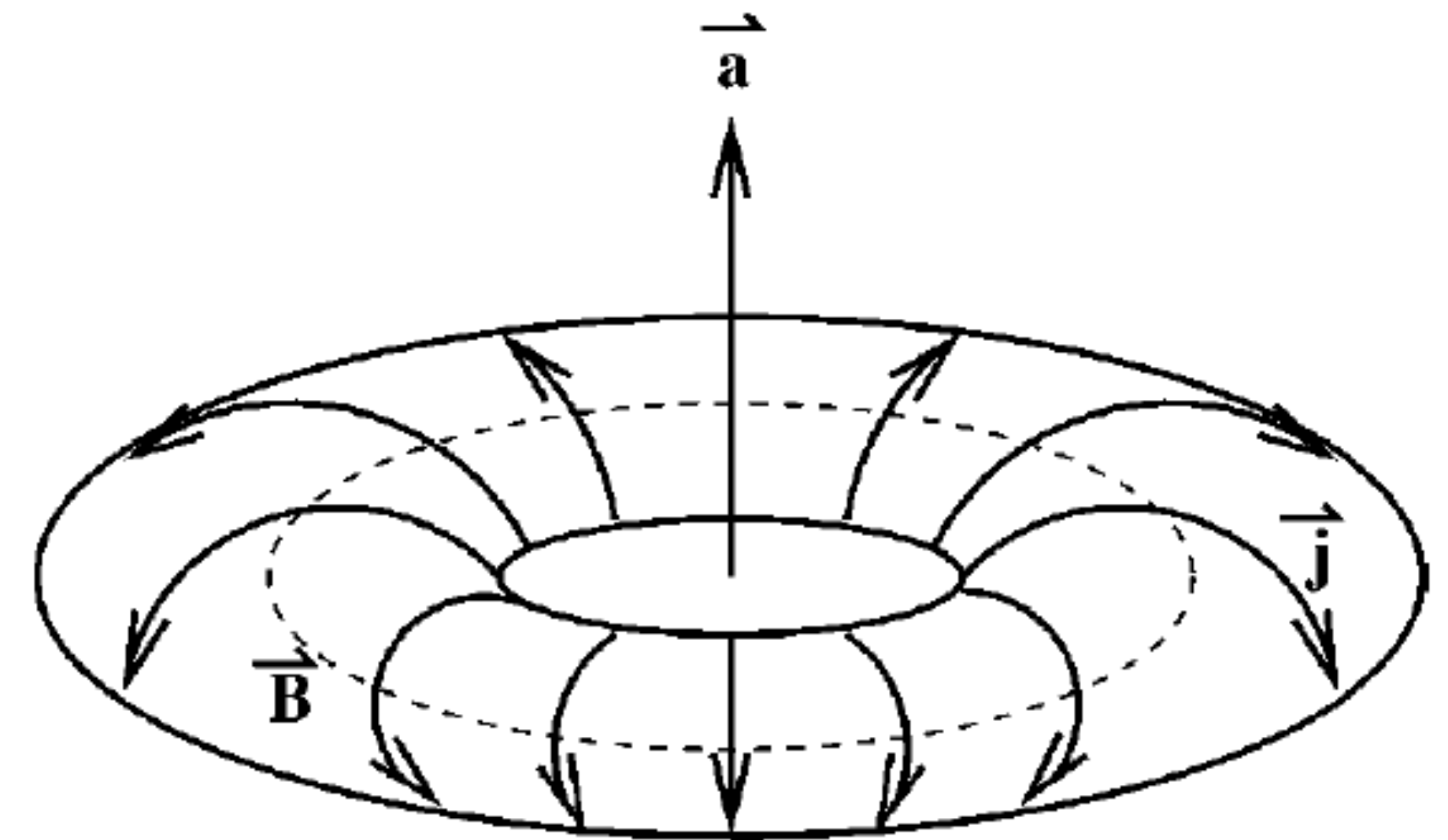
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The vector potential $\mathbf{A}^{(\text{anapole})}(\mathbf{r}) = \mu_0 \mathbf{a} \delta(\mathbf{r})$ satisfies

$$\nabla^2 \mathbf{A}^{(\text{anapole})}(\mathbf{r}) = -\mu_0 \mathbf{j}^{(\text{anapole})}(\mathbf{r})$$

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$$\mathbf{e}_{\mathbf{q}\pm 1} \equiv \mp \frac{1}{\sqrt{2}} [\mathbf{e}_x \pm i\mathbf{e}_y]$$

$$\mathbf{e}_{\mathbf{q}0} \equiv \mathbf{e}_z = \frac{\mathbf{q}}{q}$$

Anapole operator $\hat{\mathbf{a}}$ can be determined using similar expression:

$$\hat{\mathbf{a}} = \frac{1}{q^2} \hat{\mathbf{j}}^{(\text{anapole})}(\mathbf{q}) \quad \text{or} \quad \hat{a}_\lambda = \frac{1}{q^2} \hat{j}_{\mathbf{q}\lambda}^{(\text{anapole})} \quad (\lambda = 0, \pm 1).$$

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What is the expression for the anapole current operator, $\hat{j}_{\mathbf{q}\lambda}^{(\text{anapole})}$?

6

Definition of Anapole Operator

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The λ -th component of the current operator $\hat{\mathbf{j}}(\mathbf{q})$ is

$$\hat{j}_{\mathbf{q}\lambda} = -\sqrt{2\pi} \sum_{J=1}^{\infty} (-i)^J \sqrt{2J+1} \left[-\hat{T}_{J\lambda}^{\text{el}}(q) + \lambda \hat{T}_{J\lambda}^{\text{mag}}(q) \right],$$

where the transverse electric, $\hat{T}_{J\lambda}^{\text{el}}(q)$, and magnetic, $\hat{T}_{J\lambda}^{\text{mag}}(q)$, multipole operators are

$$\hat{T}_{J\lambda}^{\text{el}}(q) = \int d^3r \frac{1}{q} \nabla \times [j_J(qr) \mathbf{Y}_{JJ\lambda}(\theta, \varphi)] \cdot \hat{\mathbf{j}}(\mathbf{r}),$$

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Which multipole operator(s) should be used for $\hat{j}_{\mathbf{q}\lambda}^{(\text{anapole})}$?

7

Definition of Anapole Operator

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J	$\hat{T}_{J\lambda}^{\text{el}}(q)$	$\hat{T}_{J\lambda}^{\text{mag}}(q)$
0		
1	PT	PT
2	$P\cancel{T}$	$P\cancel{T}$
3	PT	PT
\vdots	\vdots	\vdots

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0		
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\vdots	\vdots	\vdots

The anapole current operator $\hat{j}_{\mathbf{q}\lambda}^{(\text{anapole})}$ is then given by

$$\hat{j}_{\mathbf{q}\lambda}^{(\text{anapole})} = -i\sqrt{6\pi} \hat{T}_{1\lambda}^{\text{el}}(q)$$

and the corresponding anapole operator \hat{a}_λ reads

$$\hat{a}_\lambda = \lim_{q^2 \rightarrow 0} \frac{-i\sqrt{6\pi}}{q^2} \hat{T}_{1\lambda}^{\text{el}}(q).$$

Current Conservation and Siegert's Theorem

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The transverse electric multipole operator, $\hat{T}_{J\lambda}^{\text{el}}(q)$, is given by

$$\begin{aligned} \hat{T}_{J\lambda}^{\text{el}}(q) = & -\frac{i}{q} \sqrt{\frac{J+1}{J}} \int d^3r j_J(qr) Y_{J\lambda}(\theta, \varphi) \nabla \cdot \hat{\mathbf{j}}(\mathbf{r}) \\ & - i \sqrt{\frac{2J+1}{J}} \int d^3r j_{J+1}(qr) \mathbf{Y}_{J(J+1)\lambda}(\theta, \varphi) \cdot \hat{\mathbf{j}}(\mathbf{r}). \end{aligned}$$

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Siegert's theorem:

$$\nabla \cdot \hat{\mathbf{j}}(\mathbf{r}) \doteq -\frac{1}{i\hbar} (E_i - E_f) \hat{\rho}(\mathbf{r})$$

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- ★ For the static moment, the first term is zero, but the second term is not constrained by current conservation.

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- ★ At the long-wavelength limit ($qr \rightarrow 0$), the second term vanishes, and the first term gives the correct leading-order behavior for transitions.
- ★ For the static moment, the first term is zero, but the second term is not constrained by current conservation.
- ★ This expression of $\hat{T}_{J\lambda}^{\text{el}}(q)$ is inadequate for nuclear DFT calculations because the employed current density operator is a one-body current density operator, not a many-body current density operator, so that the current conservation is not guaranteed.

Extended Siegert's theorem

J. L. Friar and S. Fallieros, PRC **29**, 1645 (1984)

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$$\hat{j}_{\mathbf{q}\eta} \doteq -\sqrt{2\pi} \sum_{J=1}^{\infty} i^J \sqrt{2J+1} \left[\hat{T}_{J\eta}^{\text{el}}(q) + \eta \hat{T}_{J\eta}^{\text{mag}}(q) \right],$$

$$\begin{aligned} \hat{T}_{J\eta}^{\text{el}}(q) &\doteq \frac{E_i - E_f}{\hbar q} \sqrt{\frac{J+1}{J}} \frac{q^J}{(2J+1)!!} \int d^3r \hat{\rho}(\mathbf{r}) r^J g_J(qr) Y_{J\eta}(\theta, \varphi) \\ &+ \frac{2q^{J+1}}{(J+2)(2J+1)!!} \int d^3r r^J \hat{\boldsymbol{\mu}}(\mathbf{r}) \cdot \mathbf{Y}_{JJ\eta}(\theta, \varphi) h_J(qr), \end{aligned}$$

$$\hat{T}_{J\eta}^{\text{mag}}(q) = 2i \sqrt{\frac{2J+1}{J+1}} \int d^3r \frac{1}{r} \hat{\boldsymbol{\mu}}(\mathbf{r}) \cdot \mathbf{Y}_{J(J-1)\eta}(\theta, \varphi) j_J(qr),$$

$$g_J(z) = 1 - \frac{Jz^2}{2(2J+3)(J+2)} \cdots \quad \text{and} \quad h_J(z) = 1 - \frac{1}{2} \frac{(J+2)z^2}{(J+4)(2J+3)} \cdots$$

Final Expression of the Anapole Operator

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For calculation of the static anapole moment, one focuses on the second term of operator $\hat{T}_{J\eta}^{\text{el}}(q)$ and simply omits the first term. Set $J = 1$, one gets

$$\hat{T}_{1\eta}^{\text{el}}(q) = -i \frac{q^2}{9} \int d^3r r^2 \left[\frac{1}{\sqrt{6\pi}} \hat{j}_\eta(\mathbf{r}) + \frac{1}{\sqrt{3}} \left[Y_2(\theta, \varphi) \otimes \hat{\mathbf{j}}(\mathbf{r}) \right]_\eta \right] \left[1 - \frac{1}{2} \frac{(J+2)(qr)^2}{(J+4)(2J+3)} \cdots \right].$$

Finally, the final expression of the anapole operator, \hat{a}_η , takes the form:

$$\begin{aligned} \hat{a}_\eta &= \lim_{q^2 \rightarrow 0} \frac{-i\sqrt{6\pi}}{q^2} \hat{T}_{1\eta}^{\text{el}}(q) \\ &= -\frac{1}{9} \int d^3r r^2 \left[\hat{j}_\eta(\mathbf{r}) + \sqrt{2\pi} \left[Y_2(\theta, \varphi) \otimes \hat{\mathbf{j}}(\mathbf{r}) \right]_\eta \right]. \end{aligned}$$

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Laboratory Anapole Moment (Work in Progress)

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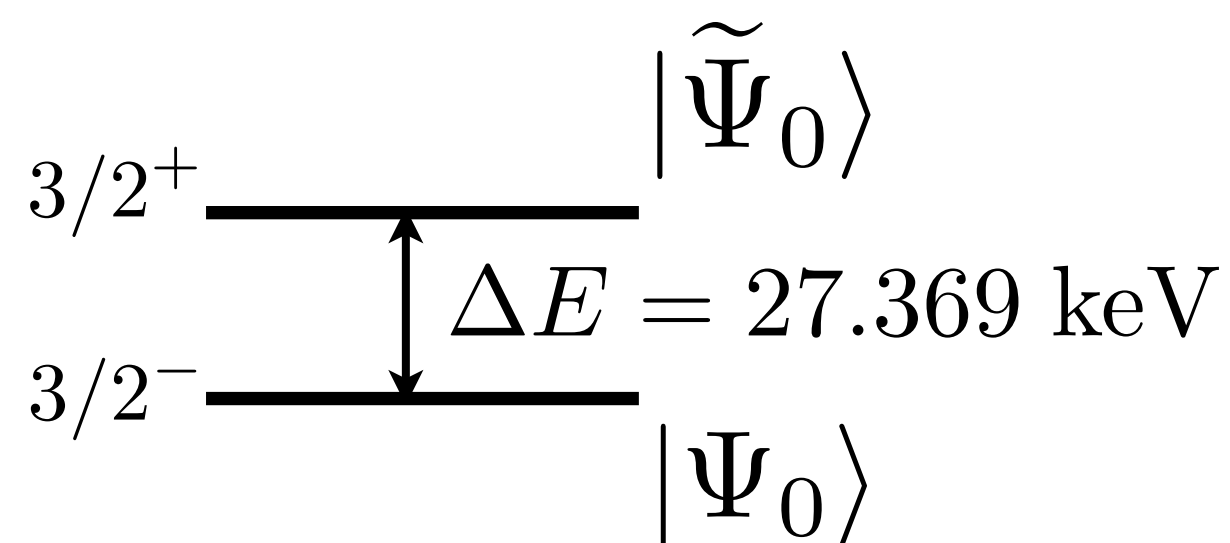
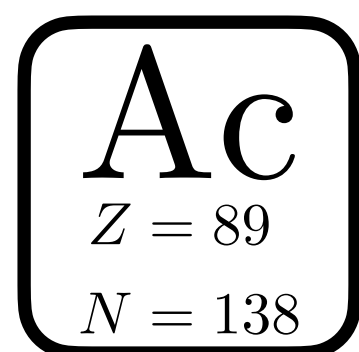
Laboratory anapole moment is calculated as

$$a_z^{\text{lab.}} \approx \sum_{i \neq 0} \frac{\langle \Psi_0 | \hat{a}_z | \Psi_i \rangle \langle \Psi_i | \hat{V}_{\text{PNC}} | \Psi_0 \rangle}{E_0 - E_i} + \text{c.c.}$$

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Ac

Z = 89

N = 138

$3/2^+$

$3/2^-$

$|\tilde{\Psi}_0\rangle$

$|\Psi_0\rangle$

$\Delta E = 27.369 \text{ keV}$

→

$a_z^{\text{lab.}}$

$\approx -2\Re$

{

$$\frac{\langle \Psi_0 | \hat{a}_z | \tilde{\Psi}_0 \rangle \langle \tilde{\Psi}_0 | \hat{V}_{\text{PNC}} | \Psi_0 \rangle}{\Delta E}$$

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3/2⁺ $|\tilde{\Psi}_0\rangle$

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Anapole operator:

$$\hat{a}_z = -\frac{1}{9} \int d^3r r^2 \left\{ \hat{j}_z(\mathbf{r}) + \sqrt{2\pi} \left[Y_2(\theta, \varphi) \otimes \hat{\mathbf{j}}(\mathbf{r}) \right]_{10} \right\}.$$

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→

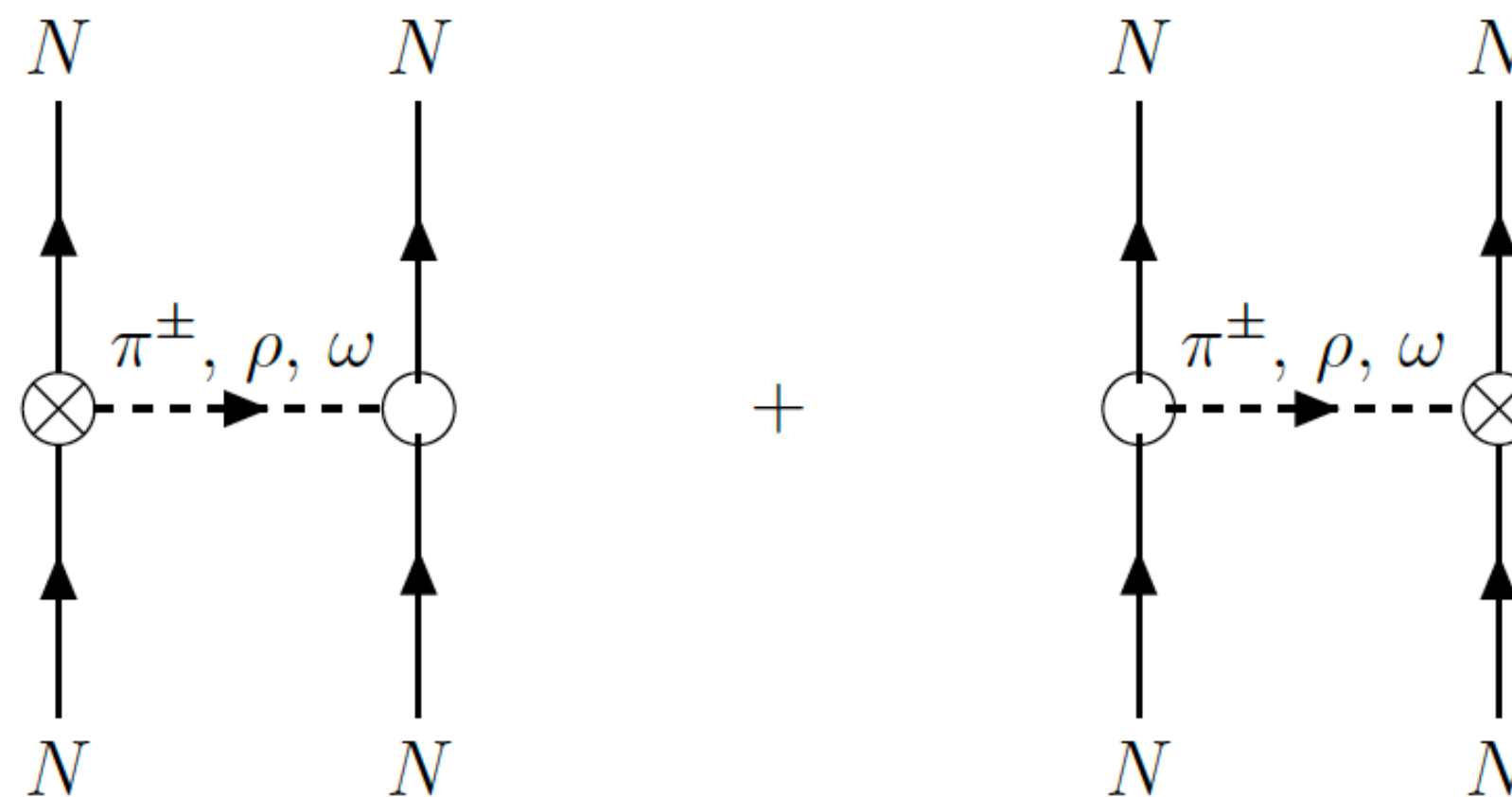
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Parity-nonconserving potential (PNC):

B. Desplanques, J. F. Donoghue, B. R. Holstein,
Ann. Phys. **124**, 449 (1980)



Summary

- ★ Nuclear anapole moments are the parity-odd and time-reversal-even E1 moments of the electromagnetic current operator.
- ★ The anapole operator derived from the extended Siegert's theorem has been chosen because there is no prescription for constructing the many-body current that guarantees current conservation.
- ★ The laboratory anapole moment is calculated using the perturbation theory, where the DDH potential is the parity-nonconserving (PNC) potential.

Outlook

- ★ To determine the intrinsic anapole moments for the isotopic chain of Actinium using different energy density functionals.
- ★ To calculate the laboratory anapole moments for octupole deformed nuclei.

Acknowledgements

We acknowledge the support from a **Leverhulme Trust Research Project Grant**. This work was partially supported by the **STFC Grant** Nos. ST/P003885/1 and ST/V001035/1 and by the **Polish National Science Centre** under Contract No. 2018/31/B/ST2/02220. We acknowledge the **CSC-IT Center for Science Ltd., Finland**, for the allocation of computational resources. This project was partly undertaken on the **Viking Cluster**, which is a high performance compute facility provided by the **University of York**. We are grateful for computational support from the **University of York High Performance Computing service, Viking and the Research Computing team**.

Back Up Slides

Parity and Time Reversal

$$\hat{T}_{J\lambda}^{\text{el}}(q) = \int d^3r \frac{1}{q} \nabla \times [j_J(qr) \mathbf{Y}_{JJ\lambda}(\theta, \varphi)] \cdot \hat{\mathbf{j}}(\mathbf{r})$$

Under the parity transformation:

$$\hat{\mathbf{j}}(\mathbf{r}) \rightarrow -\hat{\mathbf{j}}(\mathbf{r})$$

$$\nabla \rightarrow -\nabla$$

$$Y_{J\lambda}(\theta, \varphi) \rightarrow (-1)^J Y_{J\lambda}(\theta, \varphi)$$

$$\mathbf{Y}_{JJ\lambda}(\theta, \varphi) \equiv \frac{(-i\mathbf{r} \times \nabla) Y_{J\lambda}(\theta, \varphi)}{\sqrt{J(J+1)}} \rightarrow (-1)^J \mathbf{Y}_{JJ\lambda}(\theta, \varphi)$$

Therefore:

$$\hat{T}_{J\lambda}^{\text{el}}(q) \rightarrow (-1)^J \hat{T}_{J\lambda}^{\text{el}}(q)$$

$$\hat{T}_{J\lambda}^{\text{mag}}(q) = \int d^3r j_J(qr) \mathbf{Y}_{JJ\lambda}(\theta, \varphi) \cdot \hat{\mathbf{j}}(\mathbf{r})$$

Under the parity transformation:

$$\hat{T}_{J\lambda}^{\text{mag}}(q) \rightarrow (-1)^{J+1} \hat{T}_{J\lambda}^{\text{mag}}(q)$$

Under the time-reversal transformation:

$$\hat{\mathbf{j}}(\mathbf{r}) \rightarrow -\hat{\mathbf{j}}(\mathbf{r})$$

$$Y_{J\lambda}(\theta, \varphi) \rightarrow (-1)^\lambda Y_{J(-\lambda)}(\theta, \varphi)$$

$$\begin{aligned} \mathbf{Y}_{JJ\lambda}(\theta, \varphi) &\rightarrow \frac{1}{\sqrt{J(J+1)}} (+i\mathbf{r} \times \nabla) (-1)^\lambda Y_{J(-\lambda)}(\theta, \varphi) \\ &= (-1)^{\lambda+1} \mathbf{Y}_{JJ(-\lambda)}(\theta, \varphi) \end{aligned}$$

To determine the properties of the multipole operators under the time-reversal transformation, we will adhere to the convention introduced by Bohr and Mot-telson, that is:

$$\hat{\mathcal{T}}\hat{T}_{J\lambda}\hat{\mathcal{T}}^{-1} = c_{\mathcal{T}}(-1)^{J+\lambda}\hat{T}_{J(-\lambda)}$$

where $c_{\mathcal{T}}$ is the additional phase factor introduced by the time-reversal transformation.

$$\begin{aligned}\hat{T}_{J\lambda}^{\text{el}}(q) &\rightarrow \frac{1}{q} \int d^3r \nabla \times [j_J(qr)(-1)^{\lambda+1}\mathbf{Y}_{JJ(-\lambda)}(\theta, \varphi)] \cdot (-1)\hat{\mathbf{j}}(\mathbf{r}) \\ &= (-1)^{\lambda}\hat{T}_{J(-\lambda)}^{\text{el}}(q) \\ &= (-1)^{J+1}(-1)^{J+\lambda+1}\hat{T}_{J(-\lambda)}^{\text{el}}(q) \rightsquigarrow c_{\mathcal{T}} = (-1)^{J+1}\end{aligned}$$

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$$\begin{aligned}
\hat{T}_{J\lambda}^{\text{mag}}(q) &\rightarrow \int d^3r j_J(qr) (-1)^{\lambda+1} \mathbf{Y}_{JJ(-\lambda)}(\theta, \varphi) \cdot (-1) \hat{\mathbf{j}}(\mathbf{r}) \\
&= (-1)^\lambda \hat{T}_{J(-\lambda)}^{\text{mag}}(q) \\
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\end{aligned}$$

	$\hat{T}_{J\lambda}^{\text{el}}(q)$	$\hat{T}_{J\lambda}^{\text{mag}}(q)$
Parity	$(-1)^J$	$(-1)^{J+1}$
Time reversal	$(-1)^{J+1}$	$(-1)^{J+1}$