Beyond Schiff: Atomic EDMs from two-photon exchange

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Outline

- Very short review of Schiff theorem
- Multipole expansion as an expansion in powers of R_N/R_A
- 2-photon exchange appears to give larger atomic EDM than Schiff moment by 2 orders of magnitude - first, naive derivation
- Full derivation - the answer is essentially the same
- Relativistic enhancement is larger for Schiff moment (in progress)

Schiff theorem

Derivation relies on 3 assumptions:

1. Constituent particles are point-like

2. Non-relativistic dynamics

3. Only electrostatic interactions

Schiff theorem

Derivation relies on 3 assumptions: Loopholes

1. Constituent particles are point-like

   Nuclear size - Schiff moment

2. Non-relativistic dynamics

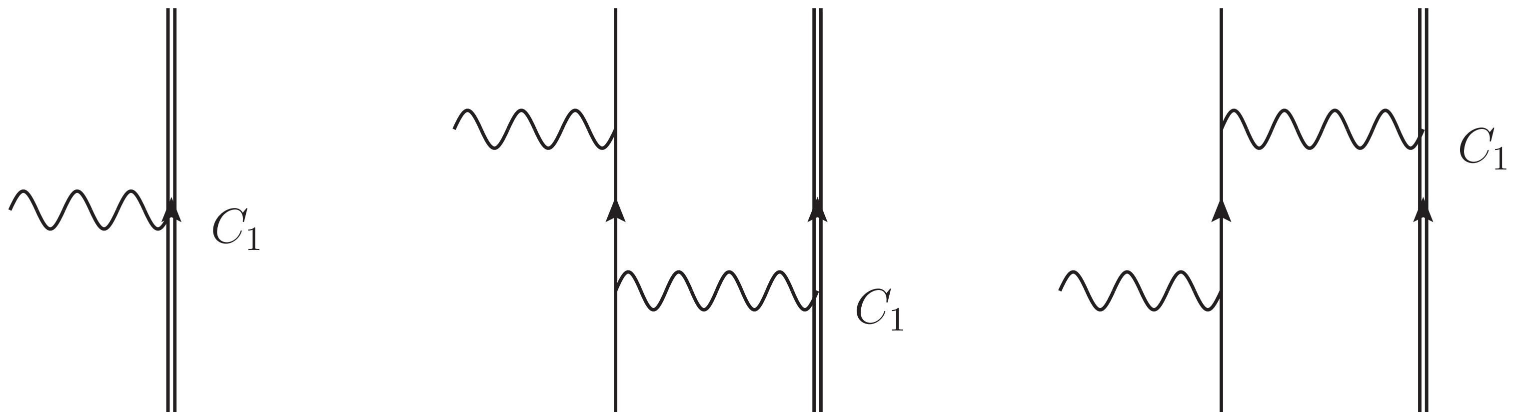
   Relativistic electrons - paramagnetic systems

3. Only electrostatic interactions

   Electromagnetic currents - topic of this talk

Natural size of interactions

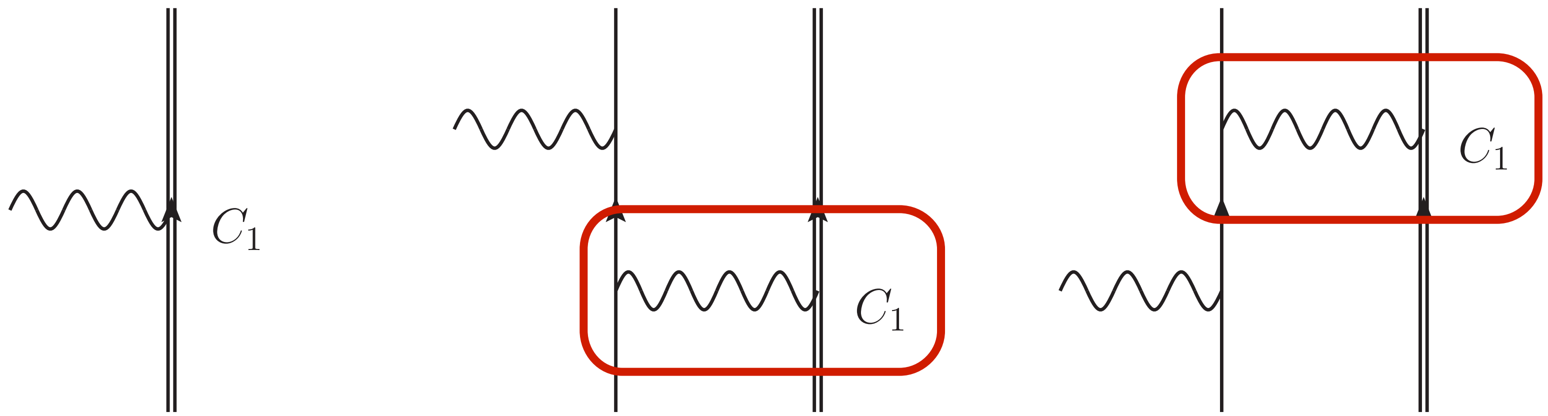
Schiff theorem is the cancellation between these diagrams



C_1 indicating that the photon couples to the nuclear EDM

Natural size of interactions

Schiff theorem is the cancellation between these diagrams



C_1 indicating that the photon couples to the nuclear EDM

Electron-nucleus interaction here is

$$V_{C1} = -\frac{4\pi\alpha}{3}\int d^3x\,\frac{\rho_e(\vec{x})}{x^2}Y_1(\hat{x})\odot\int d^3y\,y\rho_N(\vec{y})Y_1(\hat{y})$$
$$= -\boxed{\frac{4\pi\alpha}{3}\frac{R_N}{R_A^2}}C_1^A\odot C_1^N$$

lengths can be divided out

Natural size of interactions

This comes from multipole expansion of Coulomb potential

$$V_{\text{Coul}} = -\alpha \iint d^3x d^3y \frac{\rho_e(\vec{x})\rho_N(\vec{y})}{|\vec{x}-\vec{y}|}$$

Electron is usually outside the nucleus (x > y)

$$\begin{aligned}
\frac{1}{|\vec{x}-\vec{y}|} &= \sum_{lm} \frac{4\pi}{2l+1} \left(\frac{y^l}{x^{l+1}} \theta(x-y) + \frac{x^l}{y^{l+1}} \theta(y-x) \right) Y_{lm}^*(\hat{x}) Y_{lm}(\hat{y}) \\
&= \sum_{lm} \frac{4\pi}{2l+1} \left[\boxed{\frac{y^l}{x^{l+1}}} + \boxed{\left(\frac{x^l}{y^{l+1}} - \frac{y^l}{x^{l+1}} \right) \theta(y-x)} \right] Y_{lm}^*(\hat{x}) Y_{lm}(\hat{y})
\end{aligned}$$

Green terms survive in limit of point-like nucleus

l-th multipole interaction goes as $\sim \dfrac{4\pi\alpha}{R_A} \left(\dfrac{R_N}{R_A} \right)^l$

Natural size of interactions

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$$\frac{1}{|\vec{x}-\vec{y}|} = \sum_{lm} \frac{4\pi}{2l+1} \left(\frac{y^l}{x^{l+1}}\theta(x-y) + \frac{x^l}{y^{l+1}}\theta(y-x) \right) Y^*_{lm}(\hat{x}) Y_{lm}(\hat{y})$$

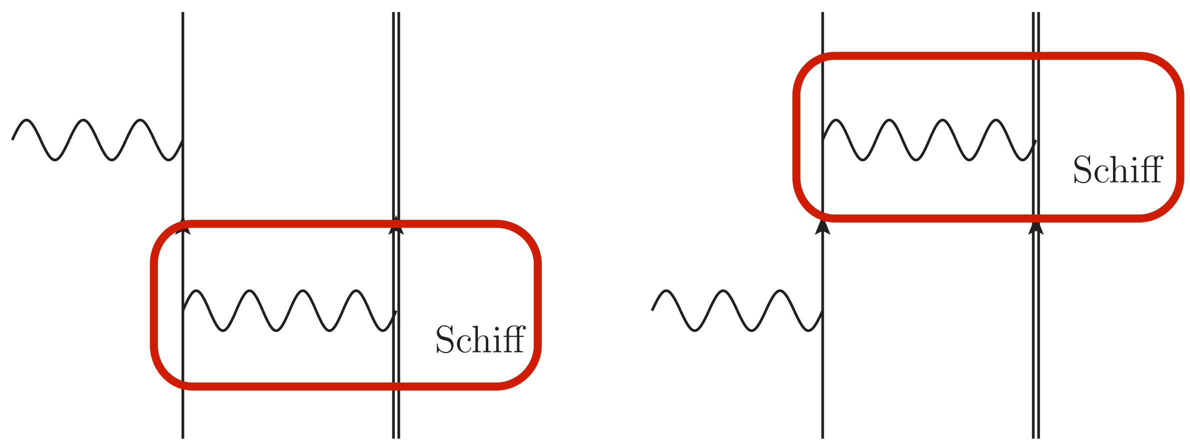
$$= \sum_{lm} \frac{4\pi}{2l+1} \left[\boxed{\frac{y^l}{x^{l+1}}} + \boxed{\left(\frac{x^l}{y^{l+1}} - \frac{y^l}{x^{l+1}} \right) \theta(y-x)} \right] Y^*_{lm}(\hat{x}) Y_{lm}(\hat{y})$$

Penetration terms are the effects of nonzero nuclear size

They are suppressed by nuclear vs atomic volume $\left(\frac{R_N}{R_A}\right)^3$

Natural size of interactions

Schiff moment contribution comes from penetration terms



Schiff moment electron-nucleus potential looks like

$$V_{\mathrm{Sch}} = \boxed{\frac{4\pi\alpha}{R_A}\left(\frac{R_N}{R_A}\right)^3}\left[R_A^4 \sum_i \left(\overleftarrow{\nabla}_i \delta^3(\vec{x}_i) + \delta^3(\vec{x}_i)\overrightarrow{\nabla}_i\right)\right] \odot \vec{S}$$

$\vec{S}$ - nuclear Schiff moment operator with lengths divided out

Volume factor - $\left(\frac{R_N}{R_A}\right)^2$ times smaller than EDM potential

Breit interaction

1-γ exchange at LO in non-relativistic expansion

$$V_{\text{Breit}} = -\alpha \iint d^3x d^3y \left[\frac{\rho_e \rho_N}{|\vec{x}-\vec{y}|} - \boxed{\frac{1}{2}\left(\frac{\vec{j}_e \cdot \vec{j}_N + (\vec{j}_e \cdot \hat{n})(\vec{j}_N \cdot \hat{n})}{|\vec{x}-\vec{y}|} \right)} \right]$$

Current-current interaction have their own multipoles

Transverse magnetic - magnetic dipole, quadrupole, etc.

$$M^N_{lm} = \int d^3y \boxed{\left(\frac{y}{R_N}\right)^l} \left[Y_l(\hat{y}) \otimes \vec{j}_N(\vec{y}) \right]_{lm}$$ note the powers of y

Transverse electric -

$$E^N_{lm} = i\sqrt{(l+1)(2l+1)} \int d^3y \boxed{\left(\frac{y}{R_N}\right)^{l-1}} \left[Y_{l-1}(\hat{y}) \otimes \vec{j}_N(\vec{y}) \right]_{lm}$$

Multipole interactions

Dividing out length scales as we did for charge multipoles,

we find the following natural sizes for multipole interactions

V_{Cl}, V_{Ml}	$\frac{4\pi\alpha}{R_A}\left(\frac{R_N}{R_A}\right)^l$
V_{El}	$\frac{4\pi\alpha}{R_A}\left(\frac{R_N}{R_A}\right)^{l-1}$
V_{Sch}	$\frac{4\pi\alpha}{R_A}\left(\frac{R_N}{R_A}\right)^3$

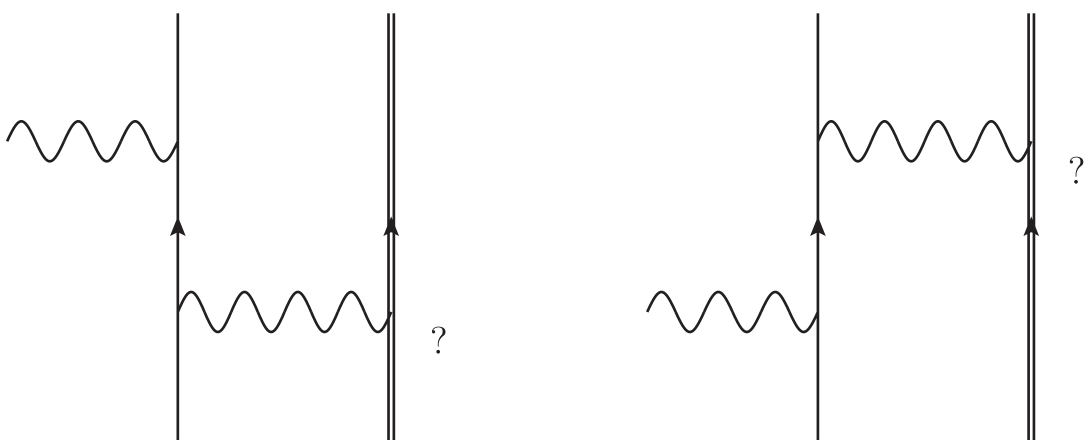
Can we find an interaction that gives a larger EDM than Schiff?

We need a PVTV effect, and as little suppression as possible

Symmetries

	$PCTC$	$PVTC$	$PCTV$	$PVTV$
C	even	—	—	odd
M	odd	—	—	even
E	—	odd	even	—

MQMs violate P and T, but



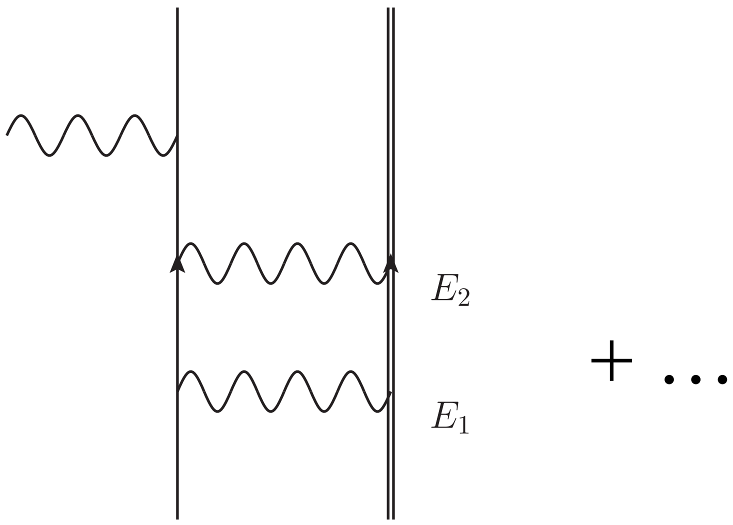
we have J=0 electronic ground state, so we can't use MQM

Schiff really is the leading contribution for 1-γ exchange

Breit iterated

	$PCTC$	$PVTC$	$PCTV$	$PVTV$
C	even	–	–	odd
M	odd	–	–	even
E	–	odd	even	–

We can go to 2-γ exchange



Combining E1 and E2 multipoles can give PVTV effect

They can also be recoupled to total J=1 (E1-M1 also possible)

Siegert's theorem

Transverse electric multipoles can be written using a gradient

$$E_{lm} = iR_N \sqrt{\frac{l+1}{l}} \int d^3y \vec{\nabla} \left[\left(\frac{y}{R_N} \right)^l Y_{lm} \right] \cdot \vec{j}_N$$

Partial integration makes $\vec{\nabla} \cdot \vec{j}_N$ appear,

which is equal to $d\rho_N/dt$ by current conservation

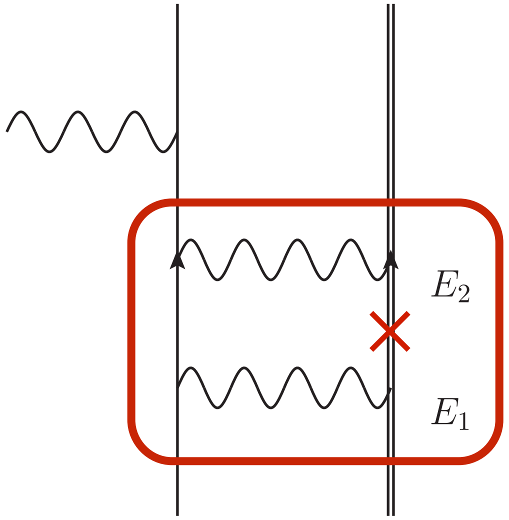
Final result is $$E_{lm} = \sqrt{\frac{l+1}{l}} R_N [C^N_{lm}, H_N]$$

where H_N is the nuclear Hamiltonian.

This shows that these multipoles have no diagonal M.E.'s

Transverse electric multipoles

Transverse electric multipoles have no static nuclear moments



nuclear excitation

In order to compare the effects of E1-E2 combination with Schiff,

we should compare using a nuclear energy denominator

$$V^{\mathrm{eff}}_{E1-E2} \sim V_{E1} \frac{1}{E_0 - E_n} V_{E2}$$

Naive comparison

So the E1-E2 effective interaction has size

$$V^{\mathrm{eff}}_{E1-E2} \sim V_{E1} \frac{1}{E_0 - E_n} V_{E2} \sim \frac{4\pi\alpha}{R_A} \cdot \frac{1}{\Delta E_N} \cdot \frac{4\pi\alpha}{R_A} \frac{R_N}{R_A}$$
$$= (4\pi\alpha)^2 \frac{R_N}{\Delta E_N R_A^3}$$

Compare this with Schiff moment interaction

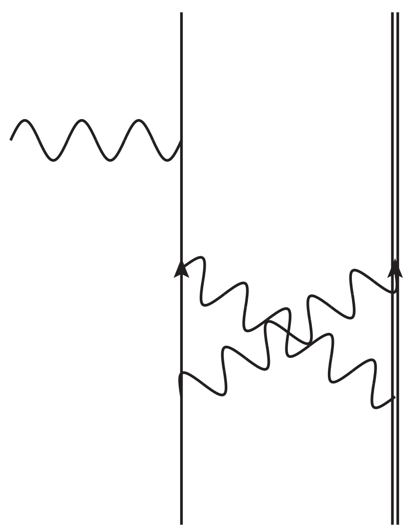
$$V_{\mathrm{Sch}} \sim (4\pi\alpha) \frac{R_N^3}{R_A^4}$$

$$\frac{V^{\mathrm{eff}}_{E1-E2}}{V_{\mathrm{Sch}}} \sim \frac{4\pi\alpha}{\Delta E_N R_N} \boxed{\frac{R_A}{R_N}}$$

E1-E2 is enhanced compared to Schiff moment!

Problems with iterating Breit

1. Crossed diagram is ignored



If electrons are relativistic, this is not small

2. Derivation of Breit interaction takes the step

$$\frac{i}{k^2} = \frac{i}{k_0^2 - \vec{k}^2} \to -\frac{i}{\vec{k}^2}$$

Not correct for inelastic scattering, which we have

Time-ordered perturbation theory

"Old-fashioned" perturbation theory, solves BOTH problems

1. Start with a normal Feynman amplitude

2. TOPT rewrites it as sum over all time-orderings of vertices

3. Propagators $\frac{i}{k^2}$ turn into energy denominators

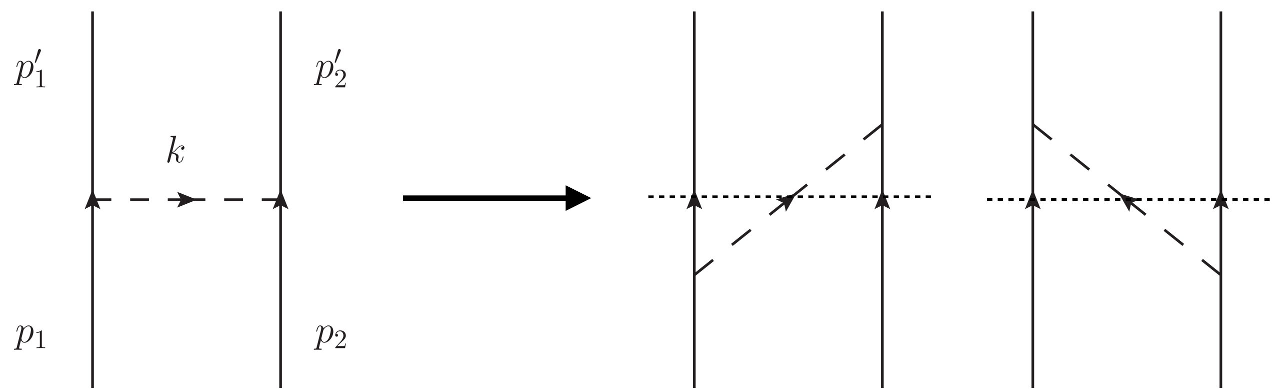
Denominators show which time-orderings are important

Also allows direct connection to non-relativistic calculation

(derivation in Sterman's QFT textbook)

Time-ordered perturbation theory

Trivial example: scalar propagator



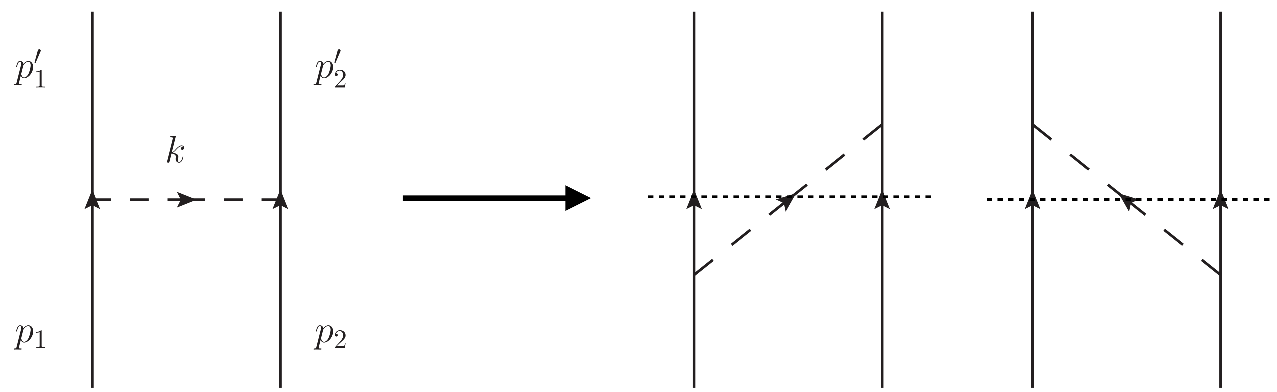
$$\frac{i}{k^2 - m^2 + i\epsilon} = \frac{1}{2\omega_{\vec{k}}}\left(\frac{i}{k^0 - \omega_{\vec{k}} + i\epsilon} - \frac{i}{k^0 + \omega_{\vec{k}} - i\epsilon}\right)$$
$$= \frac{1}{2\omega_{\vec{k}}}\left[\frac{i}{p_1^0 - (p_1'^0 + \omega_{\vec{k}}) + i\epsilon} + \frac{i}{p_2^0 - (p_2'^0 + \omega_{\vec{k}}) + i\epsilon}\right]$$

where

$$\omega_{\vec{k}} = \sqrt{\vec{k}^2 + m^2}$$

Time-ordered perturbation theory

Trivial example: scalar propagator



$$\frac{i}{k^2 - m^2 + i\epsilon} = \frac{1}{2\omega_{\vec{k}}}\left(\frac{i}{k^0 - \omega_{\vec{k}} + i\epsilon} - \frac{i}{k^0 + \omega_{\vec{k}} - i\epsilon}\right)$$

$$= \frac{1}{2\omega_{\vec{k}}}\left[\frac{i}{\boxed{p_1^0 - (p_1'^0 + \omega_{\vec{k}}) + i\epsilon}} + \frac{i}{\boxed{p_2^0 - (p_2'^0 + \omega_{\vec{k}}) + i\epsilon}}\right]$$

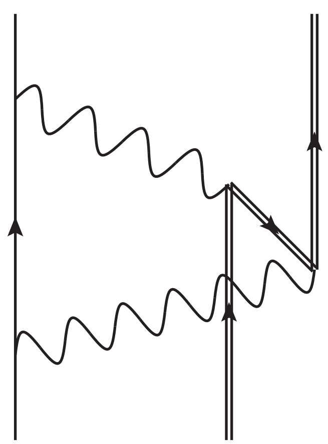
Those are energy denominators

corresponding to the 2 possible time orderings of vertices

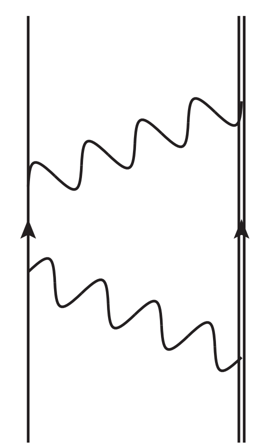
2-photon exchange in TOPT

There are 4! orderings each for box & crossed diagrams

Some orderings are highly suppressed



by particle mass



by nuclear excitation

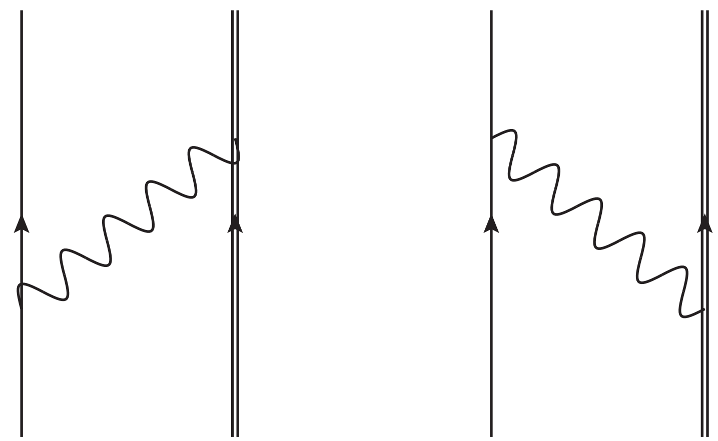
We want

1. massive particles traveling forward in time

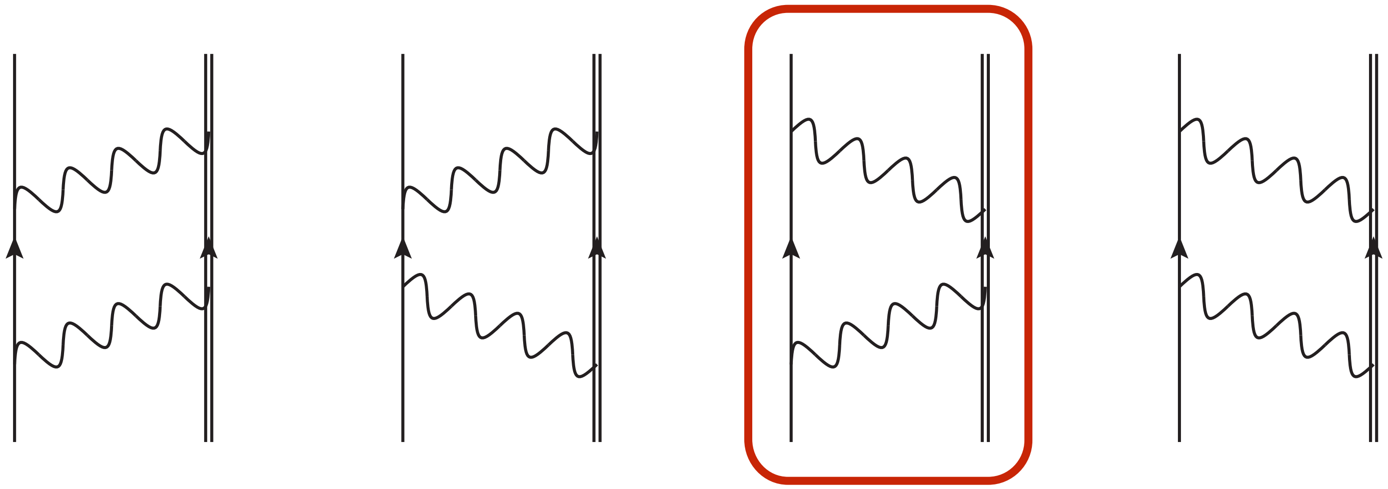
2. only 1 intermediate state with nuclear excitations

2-photon exchange in TOPT

Breit interaction comes from



Iterating Breit corresponds to assuming these 4 are leading

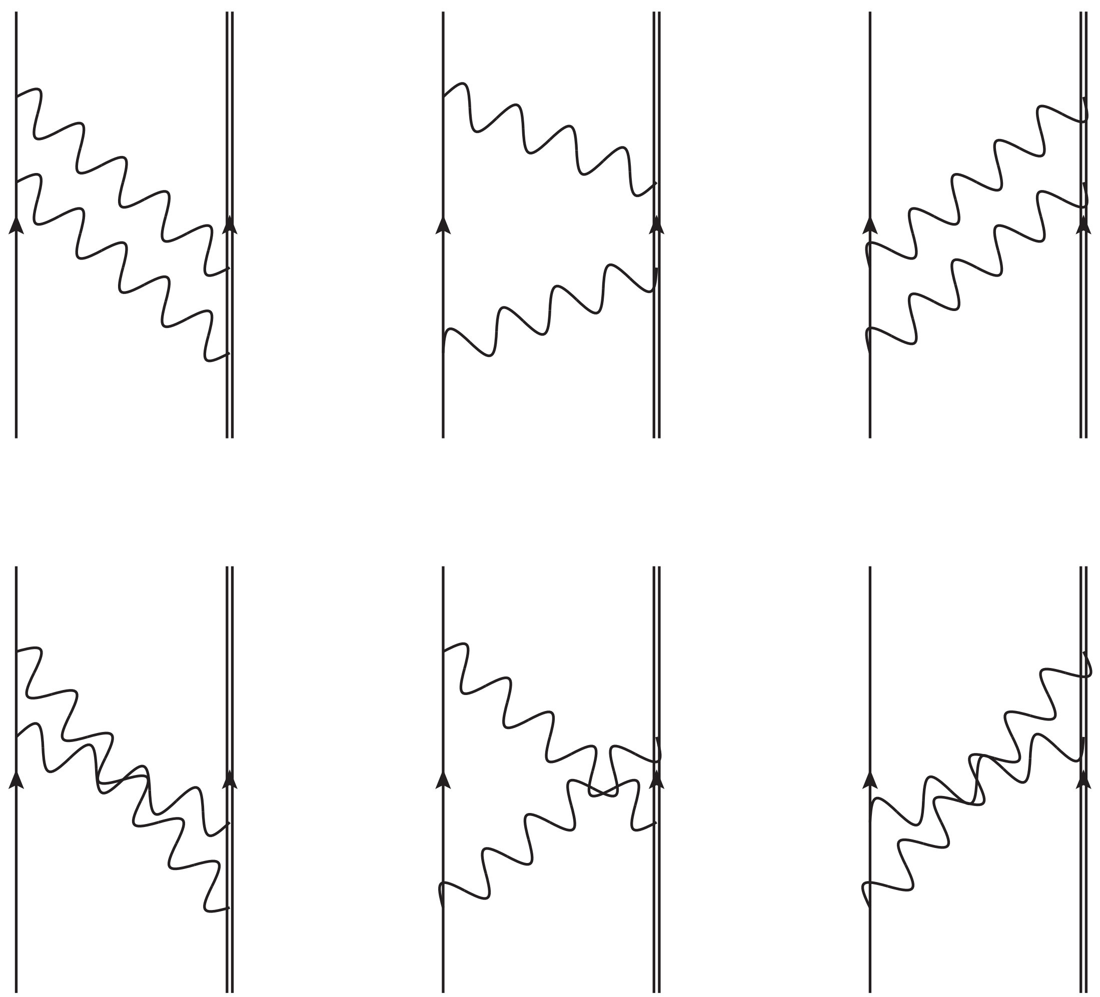


Only 1 of these is leading (1 nuclear excited state)

Adjust answer by factor of 1/4

2-photon exchange in TOPT

There are actually 6 leading diagrams - top middle is in Breit



Left and right diagrams sum to middle ones (accident?)

Crossed diagrams double the result - get back factor of 2x2 = 4

What did we learn?

This shows that the naive estimate earlier is essentially correct,

despite the incorrect use of the Breit interaction

But we do want to make a better comparison to Schiff result

1. Use Siegert's theorem and commutator trick for nuclear part

2. Relativistic enhancement near the origin

Full expression

The E1-E2 interaction is

$$V_{\text{E1-E2}} \approx \boxed{\frac{(4\pi\alpha)^2}{15\sqrt{20\pi}} \frac{R_N}{R_A^3}} \boxed{\sum_i \beta_i \left(\frac{R_A}{x_i}\right)^3 Y_1(\hat{x}_i)}$$

$$\odot \boxed{\sum_n \frac{1}{E_0 - E_n} \left\{ [\langle 0|E_1^N|n\rangle \otimes \langle n|E_2^N|0\rangle]_1 + [E_1^N \leftrightarrow E_2^N] \right\}}$$

This is to be compared with the Schiff moment interaction

$$V_{\text{Sch}} = \boxed{\frac{4\pi\alpha}{R_A}\left(\frac{R_N}{R_A}\right)^3} \boxed{\left[R_A^4 \sum_i \left(\overleftarrow{\nabla}_i \delta^3(\vec{x}_i) + \delta^3(\vec{x}_i) \overrightarrow{\nabla}_i \right) \right]} \odot \boxed{\left(\frac{\vec{S}}{R_N^3} \right)}$$

Nuclear part and electronic part can be manipulated further

Back to Siegert's theorem

Use Siegert's theorem to rewrite transverse multipoles

as commutator of charge multipoles and nuclear Hamiltonian

$$\sum_n \frac{1}{E_n - E_0} [\langle 0 | E^N_{1m_1} | n \rangle \langle n | E^N_{2m_2} | 0 \rangle + (E^N_1 \leftrightarrow E^N_2)]$$
$$= -\sqrt{3} R^2_N \sum_n (E_n - E_0) [\langle 0 | C^N_{1m_1} | n \rangle \langle n | C^N_{2m_2} | 0 \rangle + (C^N_1 \leftrightarrow C^N_2)]$$
$$= -\sqrt{3} R^2_N \langle 0 | \left[\left[C^N_{1m_1}, H_N \right], C^N_{2m_2} \right] | 0 \rangle$$

Closure sum eliminates nuclear intermediate states

Commutator

C1 and C2 can be written using nucleon coordinates;

assuming 2-body interactions are momentum-independent,

$$\sum_{m_1,m_2} \langle 0| \left[\left[C^N_{1m_1}, H_N\right], C^N_{2m_2}\right] |0\rangle \langle 10|1m_1 2m_2\rangle$$

$$= - \frac{5\sqrt{6}}{4\pi} \frac{\hbar^2}{m_N R_N^2} \boxed{\langle 0| \frac{d_{N,z}}{R_N} |0\rangle}$$

This interaction couples to the nuclear EDM,

not the Schiff moment

EDM & Schiff comparison

TABLE I. Electrodipole, Schiff, and magnetic-quadrupole moments of nuclei. The parameter η is the coefficient in the T- and P-odd interaction Hamiltonian (19). The value given in the table for the neutron was obtained from (6b) by dividing by η_n (20a).

	Nucleus	Neutron	$\frac{d}{\eta}\,[e\cdot\mathrm{cm}]\cdot 10^{21}$	$\frac{Q}{\eta}\,[e\cdot\mathrm{fm}^3]\cdot 10^{8}$	$\frac{M}{\eta}\left[\frac{e}{m_p}\cdot\mathrm{fm}\right]\cdot 10^{7}$
Outer nucleon	$^{127}I_{53}$	$p,\ d_{5/2}$	1,2	$-1{,}4$	$-1{,}4$
	$^{131}Xe_{54}$	$n,\ d_{3/2}$	0,5	$\sim 0{,}2$	$-0{,}5$
	$^{133}Cs_{55}$	$p,\ g_{7/2}$	$-0{,}9$	$+3{,}0$	1,7
	$^{135,137}Ba_{56}$	$n,\ d_{3/2}$	0,5	$\sim 0{,}2$	$-0{,}5$
	$^{147,149}Sm_{62}$	$n,\ f_{7/2}$	$-0{,}8$	$\sim 0{,}2$	2,3
	$^{201}Hg_{80}$	$n,\ p_{3/2}$	$-0{,}8$	$\sim 0{,}2$	0,8
	$^{203,205}Tl_{81}$	$p,\ s_{1/2}$	1,2	-2	–
	$^{209}Bi_{83}$	$p,\ h_{9/2}$	$-1{,}0$	3,8	2,3
spherical nuclei	$^{161}Dy_{66}$	$n,\ {}^5/_2{}^+$	7	~ 1	27
	$^{237}Np_{93}$	$p,\ {}^5/_2{}^+$	1	4	20
deformed	$^{2}H_{1}$	–	2	0	1
	$^{3}He_{2}$	–	-1	$\sim 0{,}1$	–
	light	–	$5\cdot 10^{-3}$	–	–

Sushkov, Flambaum, Khriplovich 1984

Nuclear EDM not as well calculated as Schiff moment

Note the units: d ~ $10^8\ \eta$ e fm, S ~ $10^8\ \eta$ e fm^3

Atomic enhancement

Electron wavefunctions near the origin are important

Solving Dirac equation with Coulomb potential of nucleus,

$$u_{njlm}(\vec{r}) = \begin{pmatrix} f_{njl}(r)\Omega_{jlm}(\hat{r}) \\ g_{njl}(r)(-i\vec{\sigma}\cdot\hat{r})\Omega_{jlm}(\hat{r}) \end{pmatrix}$$

with

$$f, g \sim N \frac{\boxed{Z^{1/2}}}{R_A^{3/2}} \left(\boxed{\frac{2Zr}{R_A}} \right)^{\gamma - 1}$$

$$\gamma \equiv \sqrt{(j+1/2)^2 - Z^2\alpha^2} \approx 0.8$$

Note the $Z^{1/2}$ enhancement in normalization, and

characteristic length becoming R_A/Z

Atomic enhancement

For Schiff moment,

$$\langle s_{1/2}|\vec{\nabla}\delta^3(\vec{x})|p_{1/2}\rangle$$

$$= \int d^3x\delta^3(\vec{x})(f_s^\dagger(x)f_p'(x) + g_s^\dagger(x)g_p'(x))\langle\Omega_{1/2,0}|\hat{x}|\Omega_{1/2,1}\rangle$$

$$\approx N \int d^3x\delta^3(\vec{x})\boxed{x^{2\gamma-2}}\langle\Omega_{1/2,0}|\hat{x}|\Omega_{1/2,1}\rangle$$

This is a negative power - blows up at the origin

Integral must be cut off at x = R_N. Result is ~10^5 enhancement

$$\langle s_{1/2}|\vec{\nabla}\delta^3(\vec{x})|p_{1/2}\rangle$$

$$\approx \frac{\boxed{Z^2R}}{R_A(\nu_s\nu_p)^{3/2}}\langle\Omega_{1/2,0}|\hat{x}|\Omega_{1/2,1}\rangle$$

$R \sim 10$ for large Z

Atomic enhancement

For E1-E2, $\langle s_{1/2}|\beta\frac{\hat{x}}{x^3}|p_{1/2}\rangle$

$$= \int \frac{d^3x}{x^3}(f_s^\dagger(x)f'_p(x) - g_s^\dagger(x)g'_p(x))\langle\Omega_{1/2,0}|\hat{x}|\Omega_{1/2,1}\rangle$$

$$\approx N\int dx x^{2\gamma-3}\langle\Omega_{1/2,0}|\hat{x}|\Omega_{1/2,1}\rangle = N[\boxed{x^{2\gamma-2}}]_0^{R_{\max}}$$

Same negative power, same cutoff at x = R_N.

This time, there's only 1 power of Z

$$\langle s_{1/2}|\beta\frac{\hat{x}}{x^3}|p_{1/2}\rangle$$

$$\approx \frac{\boxed{ZR}}{(\nu_s\nu_p)^{3/2}}\frac{(Z\alpha)^2}{2\gamma-2}\langle\Omega_{1/2,0}|\hat{x}|\Omega_{1/2,1}\rangle$$

Final comparison (preliminary)

Before incorporating atomic enhancement, I had 2 overall factors

$$\frac{4\pi\alpha}{10R_A}\left(\frac{R_N}{R_A}\right)^3 \text{ for Schiff moment,}$$

$$(4\pi\alpha)^2\frac{\sqrt{3}}{15\sqrt{20\pi}}\frac{\Delta E_N R_N^3}{R_A^3} \quad \text{for E1-E2,}$$

with E1-E2 being larger by ratio of ~135.

Atomic enhancement is larger for Schiff by ~Z.

E1-E2 appears to give comparable atomic EDM as Schiff moment

Conclusions

- R_N/R_A counting is a way to estimate the sizes of EDM contributions

- 2-γ exchange between electrons and the nucleus allows transverse electric multipoles to generate atomic EDM, with less R_N/R_A suppression than the Schiff moment term

- E1-E2 combination results in a coupling to the nuclear EDM, rather than the nuclear Schiff moment

- Despite the smaller relativistic enhancement, the new contribution appears comparable to Schiff. Nuclear EDM calculations are needed

Backup slides

Approximate calculation (old)

Giant dipole approximation

$$\sum_{n\neq 0}(E_n - E_0)\langle 0|C_1|n\rangle\langle n|C_2|0\rangle$$

This expression resembles

$$\sum_{n\neq 0}(E_n - E_0)|\langle 0|C_1|n\rangle|^2$$

which is known to be dominated by the giant dipole resonance.

We make the ansatz that our expression is also GDR dominated

$$\sum_{n\neq 0}(E_n - E_0)\langle 0|C_1|n\rangle\langle n|C_2|0\rangle$$

$$\approx E_{\mathrm{GDR}}\langle 0|C_1 C_2|0\rangle$$

Final expression

With these approximations, our final expression is

$$V^{\text{eff}}_{E1-E2} \approx \boxed{-(4\pi\alpha)^2 \frac{\sqrt{3}}{15\sqrt{20\pi}} \frac{E_{\text{GDR}} R_N^3}{R_A^3}} \times \boxed{\sum_{i=1}^{Z} \left(\frac{R_A}{x_i}\right)^3 Y_1(\hat{x}_i)} \odot \boxed{\{C_1^N, C_2^N\}_1}$$

We have a numerical factor, an electronic multipole, and

a nuclear multipole, which is charge dipole and quadrupole

recoupled to J=1.

Toy model calculation

We compare this nuclear moment with Schiff in a toy model

"Shell model": nucleons of ^{15}N (J=1/2) in HO potential

In order to get PVTV nuclear moments, we insert

$$V_{\mathrm{CPV}} \equiv \frac{G}{\sqrt{2}} \frac{\eta}{2m} \vec{\sigma} \cdot \vec{\nabla} \rho_{\mathrm{core}}(\vec{y})$$

as a perturbation to the HO potential, so that

$$\langle \tilde{0} | \hat{O} | \tilde{0} \rangle = \sum_{n \neq 0} \frac{\langle 0 | \hat{O} | n \rangle \langle n | V_{\mathrm{CPV}} | 0 \rangle}{E_0 - E_n} + \mathrm{c.c.}$$

is the final result.

Toy model calculation

Schiff moment has overall 1/10 in the definition

$$\vec{S} = \frac{1}{10}\int d^3y \left(\frac{y^2\vec{y}}{R_N^3} - \frac{5}{3Z}\frac{y^2\vec{d}_N}{R_N^3} \right) \rho_N(\vec{y})$$

so compare with 10 times S.

Operators	$\langle 0 \Vert \hat{O} \Vert 0 \rangle$ (normalized)
$10 \cdot S$	-10.557
$\{C_1^N, C_2^N\}_1$	11.931

Nuclear moments are the same order,

as expected from the R_N/R_A argument.

Final comparison

Comparing $$V^{\text{eff}}_{E1-E2} \approx -\boxed{(4\pi\alpha)^2 \frac{\sqrt{3}}{15\sqrt{20\pi}} \frac{E_{\text{GDR}} R_N^3}{R_A^3}}$$

$$\times \sum_{i=1}^{Z} \left(\frac{R_A}{x_i}\right)^3 Y_1(\hat{x}_i) \odot \left\{C_1^N, C_2^N\right\}_1$$

with

$$V_{\text{Sch}} = \boxed{\frac{4\pi\alpha}{10R_A}\left(\frac{R_N}{R_A}\right)^3}\left[R_A^4 \sum_i \left(\overleftarrow{\nabla}_i \delta^3(\vec{x}_i) + \delta^3(\vec{x}_i)\overrightarrow{\nabla}_i\right)\right] \odot (10\vec{S})$$

the ratio of the numerical factors is

$$\frac{4\pi\alpha}{\sqrt{15\pi}} E_{\text{GDR}} R_A \approx 135$$

taking reasonable values of $E_{\text{GDR}} = 20\,\text{MeV},\ R_A = 10^{-10}\,\text{m}$

Multipoles

Multipoles

Full expansion of Breit interaction

$$V_{Cl} = -\frac{4\pi\alpha}{(2l+1)R_A}\left(\frac{R_N}{R_A}\right)^l C_l^A \odot C_l^N$$

$$V_{Ml} = \frac{4\pi\alpha}{(2l+1)R_A}\left(\frac{R_N}{R_A}\right)^l M_l^A \odot M_l^N$$

$$V_{El} = \frac{4\pi\alpha}{(2l+1)R_A}\left(\frac{R_N}{R_A}\right)^{l-1} {E'}_l^A \odot E_l^N$$

$$V_{E'l} = \frac{4\pi\alpha}{(2l+1)R_A}\left(\frac{R_N}{R_A}\right)^{l+1} E_l^A \odot {E'}_l^N$$

There are 2 kinds of transverse electric terms,

but one is larger by R_N/R_A counting

Multipoles

List of electronic multipole operators

$$C_{lm}^{A} \equiv \int d^3x \left(\frac{R_A}{x}\right)^{l+1} \rho_e(\vec{x}) Y_{lm}(\hat{x})$$

$$M_{lm}^{A} \equiv \int d^3x \left(\frac{R_A}{x}\right)^{l+1} \vec{Y}_{lm}^{l}(\hat{x}) \cdot \vec{j}_e(\vec{x})$$

$$E_{lm}^{A} \equiv R_A^{l+2} \int d^3x \left[\vec{\nabla} \times \left(\frac{1}{x^{l+1}} \vec{Y}_{lm}^{l}(\hat{x})\right)\right] \cdot \vec{j}_e(\vec{x})$$

$$E_{lm}^{\prime A} \equiv R_A^{l} \int d^3x \left[\vec{\nabla} \times \left(\frac{1}{2(2l-1)x^{l-1}} \vec{Y}_{lm}^{l}(\hat{x})\right)\right] \cdot \vec{j}_e(\vec{x})$$

E′ is the relevant transverse electric operator

Multipoles

List of nuclear multipole operators

$$C_{lm}^{N} \equiv \int d^3y \left(\frac{y}{R_N}\right)^l \rho_N(\vec{y}) Y_{lm}(\hat{y})$$

$$M_{lm}^{N} \equiv \int d^3y \left(\frac{y}{R_N}\right)^l \vec{Y}_{lm}^{l}(\hat{y}) \cdot \vec{j}_N(\vec{y})$$

$$E_{lm}^{N} \equiv \frac{1}{R_N^{l-1}} \int d^3y \left[\vec{\nabla} \times \left(y^l \vec{Y}_{lm}^{l}(\hat{y})\right)\right] \cdot \vec{j}_N(\vec{y})$$

$$E_{lm}^{\prime N} \equiv \frac{1}{R_N^{l+1}} \int d^3y \left[\vec{\nabla} \times \left(-\frac{y^{l+2}}{2(2l+3)} \vec{Y}_{lm}^{l}(\hat{y})\right)\right] \cdot \vec{j}_N(\vec{y})$$

E is the relevant transverse electric operator

Time reversal

Time reversal

Multipoles are either parity even or odd

even: total charge (monopole), magnetic dipole, etc.

odd: EDM, magnetic quadrupole, etc.

Properties of operators under time reversal is more subtle,

especially when we consider products of operators.

Time reversal

The starting point is the relation $\langle T\psi | T\phi\rangle = \langle\phi|\psi\rangle$

Notice that the bra and ket get reversed.

Consider EDM in T conservation limit:

$$\begin{aligned}\langle jj|C^N_{10}|jj\rangle &= \left[TC^N_{10}|jj\rangle\right]^\dagger (T|jj\rangle) \\ &= \left[C^N_{10} i^{2j}|j,-j\rangle\right]^\dagger (i^{2j}|j,-j\rangle) \\ &= \langle j,-j|C^N_{10}|j,-j\rangle\end{aligned}$$

Wigner-Eckart relates these by a minus sign -> no EDM

Another way to say this: C^N_1 does not behave like spin under T

Time reversal

For J=1 operators, TV moments come from operators

that behave in the same way under T and complex conjugation

$\hat{O}$	$T\hat{O}T^{-1}$	$\hat{O}^\dagger$
C^N_{1m}	$(-1)^m C^N_{1,-m}$	$(-1)^m C^N_{1,-m}$
M^N_{1m}	$(-1)^m M^N_{1,-m}$	$(-1)^{m+1} M^N_{1,-m}$
E^N_{1m}	$(-1)^m E^N_{1,-m}$	$(-1)^{m+1} E^N_{1,-m}$
$\{E_1, E_2\}^N_{1m}$	$(-1)^m \{E_1, E_2\}^N_{1,-m}$	$(-1)^m \{E_1, E_2\}^N_{1,-m}$
$[E_1, E_2]^N_{1m}$	$(-1)^m [E_1, E_2]^N_{1,-m}$	$(-1)^{m+1} [E_1, E_2]^N_{1,-m}$
$\{E_1, M_1\}^N_{1m}$	$(-1)^{m+1} \{E_1, M_1\}^N_{1,-m}$	$(-1)^{m+1} \{E_1, M_1\}^N_{1,-m}$
$[E_1, M_1]^N_{1m}$	$(-1)^{m+1} [E_1, M_1]^N_{1,-m}$	$(-1)^m [E_1, M_1]^N_{1,-m}$

Time reversal

Multipoles are either parity even or odd

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Properties of operators under time reversal is more subtle,

especially when we consider products of operators.

Time-ordered perturbation theory

Time-ordered perturbation theory

Steps to the derivation:

1. Write the energy-conserving delta functions at each vertex as

$$\delta(p^0_{\text{in}} - p^0_{\text{out}}) = \int_{-\infty}^{\infty} dt\, e^{i(p^0_{\text{in}} - p^0_{\text{out}})t}$$

If an internal line, k, starts at vertex with time t_i

and ends at vertex with time t_j, then there is a factor

$$e^{ip^0_k(t_j - t_i)}$$

Time-ordered perturbation theory

2. This factor, $e^{ip_k^0(t_j - t_i)}$, lets us do the integration over p_k^0

by closing the contour at infinity.

Contour integral picks up a pole from the propagator of this line,

and the pole corresponds to the on-shell energy of the particle.

Result:

$$\int \frac{d^4p}{(2\pi)^4} \rightarrow \int \frac{d^3p}{(2\pi)^3 2\omega_{\vec{k}}}$$

Any function of k^0 in the numerator is evaluated

with on-shell energy, since that gives the residue

Time-ordered perturbation theory

3. We still have time integrals that we introduced at the start.

The integrand is now $e^{i(E_{\mathrm{in}}-E_{\mathrm{out}})t}$ with on-shell energies.

But whether the particle is 'in' or 'out' depends on

the time ordering of the vertices.

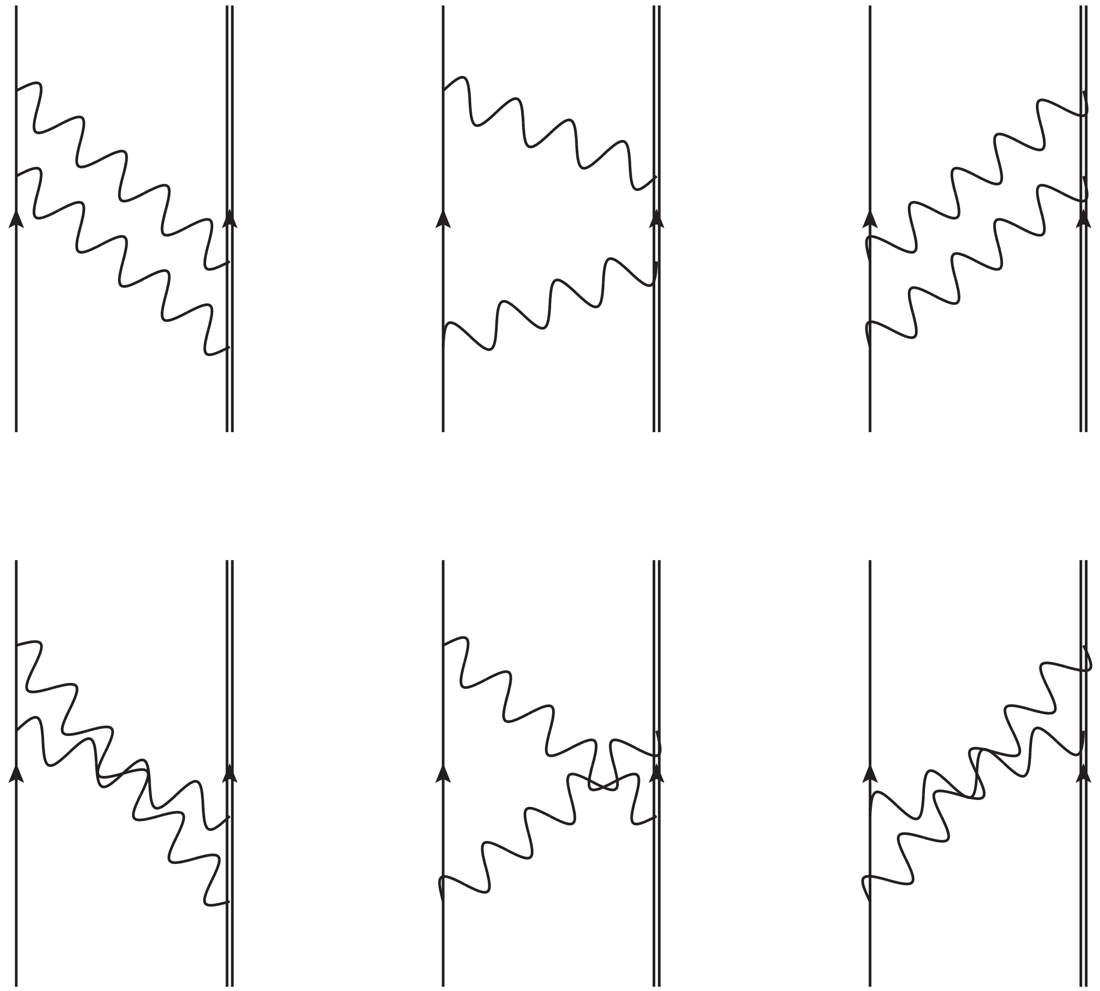
Split up the integral into regions, which correspond to orderings.

Then we can perform the integrals fully.

Result: an energy denominator for each intermediate state

Time-ordered perturbation theory

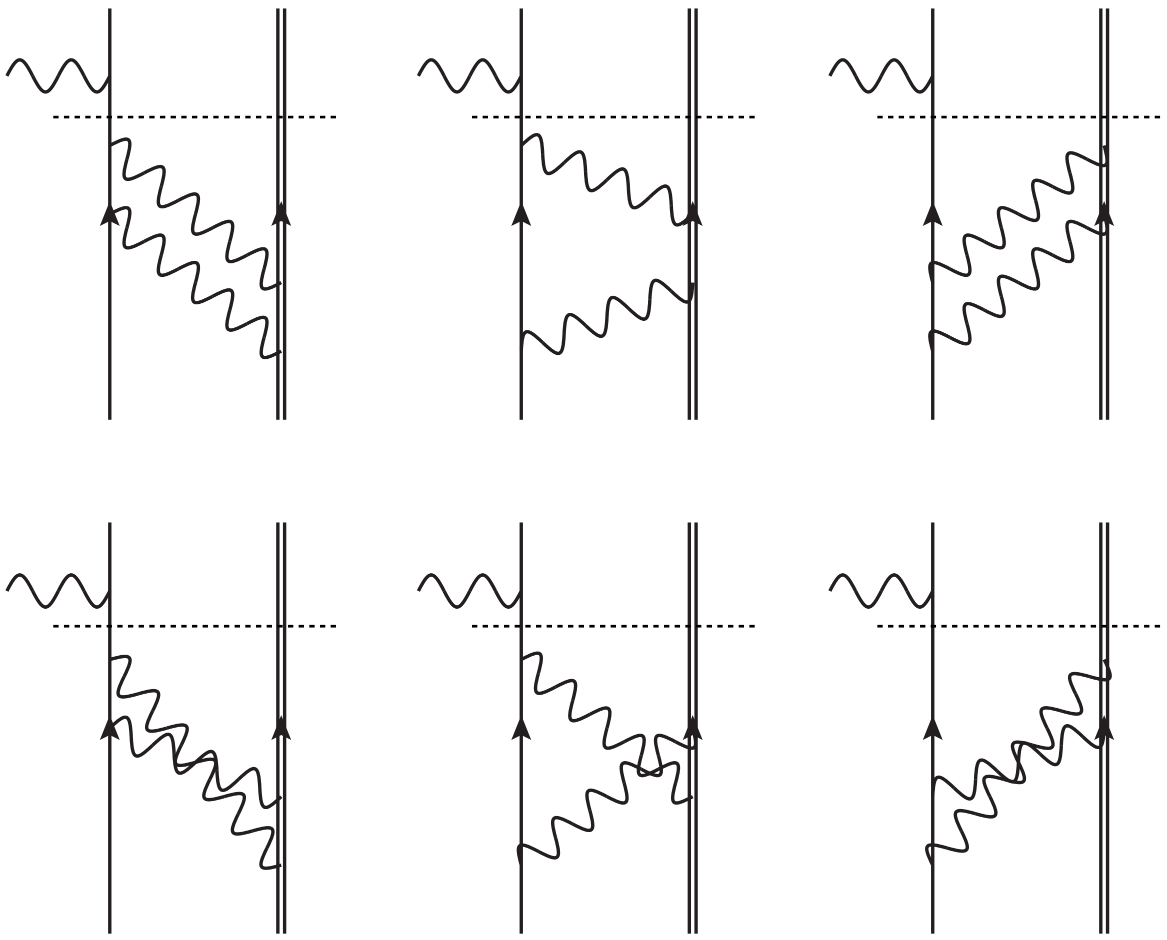
Why is it sufficient to consider



Justification comes from TOPT

Time-ordered perturbation theory

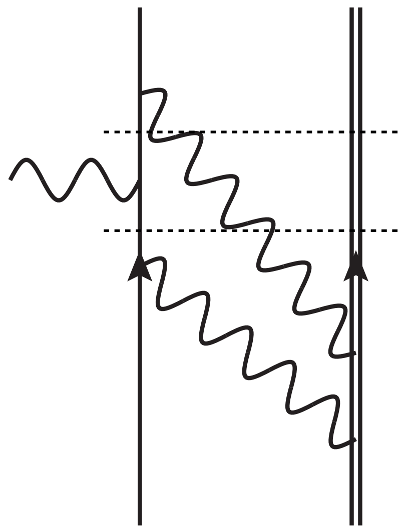
These have a pure atomic excitation as the last intermediate state



Compare with…

Time-ordered perturbation theory

…for example



This diagram has massive particles always traveling forward,

and only 1 nuclear excitation.

But atomic excited state always appears with a photon,

which makes the denominator not so small