Nonrelativistic QED

for bound state theory in Quantum Electrodynamics

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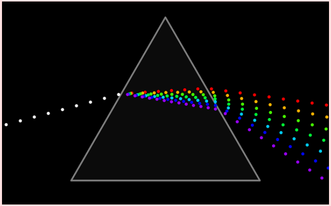

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Nonrelativistic QED

Concept of NRQED

QED

$$\mathcal{L}_{\mathrm{QED}} = \bar{\psi}\left[(i\partial - e\,A)\,\gamma - m\right]\psi - \frac{1}{4}F_{\mu\nu}F^{\mu\nu},$$

$$\Downarrow$$

Nonrelativistic QED

$$\mathcal{L}_{\mathrm{NRQED}}$$

$$\Downarrow$$

Effective Hamiltonian

$$H_{\mathrm{eff}} = \sum_i \frac{\mathbf{P}_i^2}{2m_i} + e^2 \sum_{j>i} \frac{Z_i Z_j}{r_{ij}} + \text{higher order corrections}$$

(Here $\mathbf{P}_i = \mathbf{p}_i + e\mathbf{A}$)

Nonrelativistic QED Lagrangian

The Lagrangian for NRQED is built out nonrelativistic (two-component) Pauli spinor fields ψ for each of the electron, positron, muon, proton, etc. Photons are treated in the same fashion as in QED.

$$
\begin{aligned}
L_{\rm eff} = & -\frac{1}{2}(E^2 - B^2) + \psi_e^* \left(i\partial_t - e\varphi + \frac{\mathbf{D}^2}{2m} + \frac{\mathbf{D}^4}{8m^3} + \dots \right) \psi_e \\
& + \psi_e^* \left(c_F \tfrac{e}{2m} \boldsymbol{\sigma}\mathbf{B} + c_D \tfrac{e}{8m^2} \left[\mathbf{DE}\right] + c_S \tfrac{e}{8m^2} \left\{ \boldsymbol{\sigma} \cdot [i\mathbf{D} \times \mathbf{E}] \right\} \right) \psi_e \\
& + \text{higher order terms} + \text{muon, proton, etc.} \\
& - \tfrac{d_1}{m_e m_\ell} (\psi_e^* \boldsymbol{\sigma}_e \psi_e)(\psi_\ell^* \boldsymbol{\sigma}_\ell \psi_\ell) + \tfrac{d_2}{m_e m_\ell} (\psi_e^* \psi_e)(\psi_\ell^* \psi_\ell) + \dots
\end{aligned}
$$

where $\mathbf{D} = \boldsymbol{\nabla} - ie\mathbf{A}$.

Wilson coefficients

Wilson coefficients for the electron interactions with external field:

$$c_D = 1 + 2\kappa + \frac{\alpha}{\pi}\frac{8}{3}\left[\ln\left(\frac{m}{2\Lambda}\right) + \frac{5}{6} - \frac{3}{8}\right],$$

$$c_S = 1 + 2\kappa,$$

$$c_F = 1 + \kappa.$$

Wilson coefficients for contact interactions:

$$d_1 = (Z\alpha)^2 \frac{2}{m_e^2 - m_\ell^2} \ln\left(\frac{m_e}{m_\ell}\right),$$

$$d_2 = (Z\alpha)^2 \left\{\frac{7}{3} - 2\ln\left(\frac{m}{2\Lambda}\right) + \frac{2}{m_e^2 - m_\ell^2}\left[m_e^2 \ln\left(\frac{m_\ell}{\mu}\right) - m_\ell^2 \ln\left(\frac{m_e}{\mu}\right)\right]\right\}.$$

NRQED requirements

Requirements for the NRQED Lagrangian interaction terms:

- Hermiticity;
- Gauge invariance. We use covariant derivatives: $\mathbf{D} = \boldsymbol{\nabla} - ie\mathbf{A}$;
- Parity. The Lagrangian should be parity even;
- Time reversal. The Lagrangian should be even under time reversal transformation.
- Coupling constants are determined by requiring that predictions of QED and NRQED agree to a desired order in (v/c);
- Contributions from QED that involve relativistic loop momenta are absorbed into NRQED in a form of various local interactions.

Following[1] we use operators: $iD_t, i\mathbf{D}, \mathbf{B}, \mathbf{E}, \boldsymbol{\sigma}$, as building blocks of the Lagrangian and expand it into a series of inverse powers of the electron mass m:

$$\mathcal{L} = \sum_{n=0} \psi_e^* \frac{O_n}{m^n} \psi_e.$$

	$i\mathbf{D}$	$\mathbf{E}$	$\mathbf{B}$	$\boldsymbol{\sigma}$
P	$-$	$-$	$+$	$+$
T	$-$	$+$	$-$	$-$
	M^1	M^2	M^2	M^0

Spatial parity and time reversal symmetries, and mass dimension of operators.

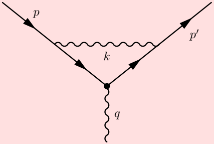
[1] Gil Paz. *An introduction to NRQED*. Modern Physics Letters A. **30**, 1550128 (2015).

Lagrangian NRQED

Using symmetries imposed on the Lagrangian, one can show that the form $\mathcal{L}$ **is unique**, and the coefficients: c_F, c_D, etc. can be unambiguously obtained from a comparison with the scattering amplitude in QED after choosing the NRQED regularization method.

The only arbitrariness remains with the ambiguity of choosing a basis for homogeneous polynomials:

$$p^2 + p'^2, \quad \mathbf{pp}' \qquad \text{or} \qquad (\mathbf{p}+\mathbf{p}')^2, \quad (\mathbf{p}-\mathbf{p}')^2$$

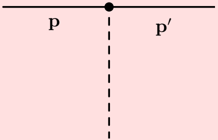


Basic interactions and perturbation theory

Examples of basic interactions in NRQED. Vertices.

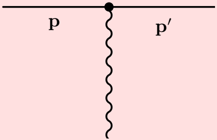
Coulomb

e



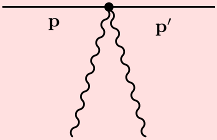
"dipole"

$-e\left[\frac{\mathbf{p}'+\mathbf{p}}{2m}\right]$



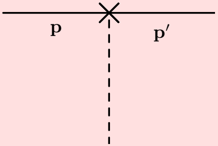
$\mathbf{A}^2$

$e^2\left[\frac{\delta^{ij}}{2m}\right]$



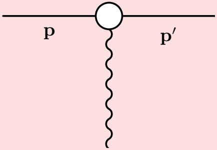
Darwin's

$-e\left[\frac{1}{8m^2}\right]\mathbf{q}^2$



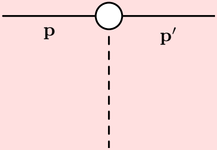
Fermi's

$e\left[\frac{i}{2m}\right](\mathbf{q}\times\boldsymbol{\sigma})$



spin–orbit

$e\left[\frac{i}{4m^2}\right](\mathbf{p}'\times\mathbf{p})\cdot\boldsymbol{\sigma}$



Here $\mathbf{q}=\mathbf{p}'-\mathbf{p}$ is a transferred impulse of the particle.

NRQED propagators

A natural choice of a gauge for the electromagnetic field is the **Coulomb gauge** ($\mathbf{kA} = 0$)

$$\begin{cases} G^{00} = \dfrac{1}{\mathbf{k}^2}\,, & \text{— the Coulomb photon propagator,} \\[2ex] G^{ij} = \dfrac{\delta_{ij} - k_i k_j/\mathbf{k}^2}{k^2 + i\varepsilon}\,, & \text{— the transverse photon propagator,} \\ G^{0i} = G^{i0} = 0, \qquad i,j = 1,2,3. & \end{cases}$$

Propagators for massive particles

$$\frac{1}{E - \mathbf{p}^2/(2m) + i\varepsilon}\,.$$

Zero-order approximation

Zero-order Lagrangian is

$$L^{(0)}_{\rm eff} = -\frac{1}{2}(E^2 - B^2) + \sum_n \psi_n^* \left(i\partial_t - eZ_n\varphi + \frac{\mathbf{D}^2}{2m_n} \right) \psi_n \,.$$

By variation of field functions ψ_n and quantization of the electromagnetic field, one gets the nonrelativistic Hamiltonian of a system of particles interacting with an electromagnetic field:

$$\breve{H}_0 = \sum_i \frac{\mathbf{P}_i^2}{2m_i} + e^2 \sum_{j>i} \frac{Z_iZ_j}{r_{ij}} + \sum_{\lambda=1,2} \int d^3k\, k\, a^+_{k\lambda} a_{k\lambda}. \qquad (*)$$

Here $\mathbf{P}_i = \mathbf{p}_i + eZ_i\mathbf{A}$. Operators $\mathbf{A}(\mathbf{r})$ are presented in terms of photon creation and annihilation operators

$$\mathbf{A}(\mathbf{r}) = (2\pi)^{-3/2} \int \frac{d^3k}{\sqrt{2k}} \left(a^+_{k\lambda} e^{-i\mathbf{kr}} + a_{k\lambda} e^{i\mathbf{kr}} \right) \mathbf{e}_\lambda.$$

Hamiltonian (*) is a convenient starting point for building up the nonrelativistic quantum electrodynamics (NRQED) in the Hamiltonian form.

Nonstationary perturbation theory

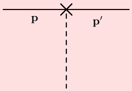
Let $H = H_0 + V$, then we can expand K in increasing powers of V:

$$K(2,1) = K_0(2,1) + K^{(1)}(2,1) + K^{(2)}(2,1) + \dots$$

where $K_0(2,1)$ is a propagator (or a Green's function) of the unperturbed Hamiltonian:

$$K_0(2,1) = e^{-iH_0(t_2-t_1)},$$
$$[i\partial/\partial t_2 - H_0(2)]\, K_0(2,1) = i\delta(2,1).$$

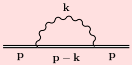
For instantaneous interaction:



$$K^{(1)}(2,1) = -i \int K_0(2,3)V(3)K_0(3,1)\, d\tau_3,$$

For a transverse photon:

$$K^{(1)}(2,1) = -i \int K_0(2,4)V(4)G(4,3)K_0(4,3)V(3)K_0(3,1)d\tau_3 d\tau_4,$$



Functions $V(3)$ and $V(4)$ are some vertex functions of interaction with the electro-magnetic field.

Perturbation theory for a stationary state

$$\Delta E = \int \prod_i^N d\mathbf{r}'_i \prod_j^N d\mathbf{r}_j \, d(t'-t) \, \frac{1}{(2\pi)^4} \int d^4k \, \psi_0^*(\mathbf{r}_j,t) V(2)$$
$$\left\{ e^{-i(k_0 t - \mathbf{k}\mathbf{r}_j)} \left[\frac{4\pi}{k^2+i\epsilon} \left(\delta_{ij} - \frac{k_i k_j}{\mathbf{k}^2} \right) \right] e^{i(k_0 t' - \mathbf{k}\mathbf{r}_i)} \, K_0(2,1) \right\} V(1) \psi_0(\mathbf{r}_i, t')$$

Integrating over t one gets

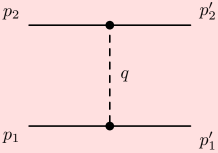
$$\Delta E = \frac{1}{(2\pi)^4 \, i} \int \frac{d^4k}{k^2+i\epsilon} 4\pi \left(\delta_{ij} - \frac{k_i k_j}{\mathbf{k}^2} \right) \left\langle \psi_0 \left| V(2) \, e^{i\mathbf{k}\mathbf{r}_a} \frac{1}{E_0 - k_0 - H_0} e^{-i\mathbf{k}\mathbf{r}_b} \, V(1) \right| \psi_0 \right\rangle - \delta_{ab} \, \delta m \, \langle \psi_0 | \psi_0 \rangle$$

or performing integration over k_0 ($k = |\mathbf{k}|$):

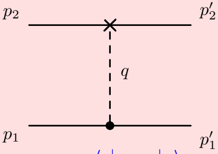
$$\Delta E = \frac{1}{(2\pi)^3} \int \frac{d^3\mathbf{k}}{2k} 4\pi \left(\delta_{ij} - \frac{k_i k_j}{\mathbf{k}^2} \right) \left\langle \psi_0 \left| V(2) \, e^{i\mathbf{k}\mathbf{r}_a} \frac{1}{E_0 - k - H_0} e^{-i\mathbf{k}\mathbf{r}_b} \, V(1) \right| \psi_0 \right\rangle - \delta_{ab} \, \delta m \, \langle \psi_0 | \psi_0 \rangle$$

Leading order relativistic and radiative contributions.

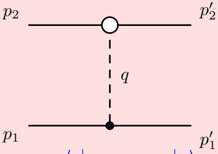
Breit-Pauli Hamiltonian



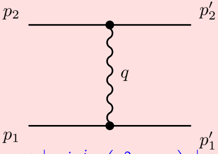
$$e^2 \left\langle i \left| \frac{1}{\mathbf{q}^2} \right| f \right\rangle$$



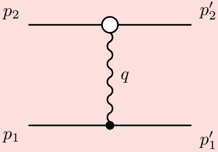
$$-e^2\, c_D^{(2)} \left\langle i \left| \frac{1}{8m_2^2} \right| f \right\rangle$$



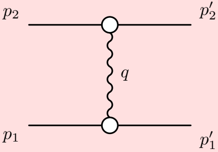
$$e^2\, c_S^{(2)} \left\langle i \left| \frac{i\boldsymbol{\sigma}_2[\mathbf{q}\times\mathbf{p}_2]}{4m_2^2\mathbf{q}^2} \right| f \right\rangle$$



$$-e^2 \left\langle i \left| \frac{p_1^i p_2^j}{m_1 m_2} \left(\frac{\mathbf{q}^2 - q_i q_j}{\mathbf{q}^4} \right) \right| f \right\rangle$$



$$e^2\, c_F^{(2)} \left\langle i \left| \frac{i\boldsymbol{\sigma}_2[\mathbf{q}\times\mathbf{p}_1]}{2m_1 m_2\mathbf{q}^2} \right| f \right\rangle$$



$$-e^2\, c_F^{(1)}\, c_F^{(2)} \left\langle i \left| \frac{[\mathbf{q}\times\boldsymbol{\sigma}_1][\mathbf{q}\times\boldsymbol{\sigma}_2]}{4m_1 m_2\mathbf{q}^2} \right| f \right\rangle$$

Breit-Pauli Hamiltonian in the coordinate space

Taking into account the relativistic correction to the kinetic energy

$$E = c\sqrt{m^2c^2+\mathbf{p}^2} = mc^2 + \mathbf{p}^2/2m + \mathbf{p}^4/8c^2m^3 + \dots$$

The Breit-Pauli Hamiltonian takes a form ($\mathbf{r}_{ij} = \mathbf{r}_j - \mathbf{r}_i$):

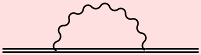
$$H_B = -\frac{1}{c^2}\sum_i \frac{\mathbf{p}_i^4}{8m_i^3} + U_B,$$

$$U_B = -\frac{e^2}{c^2}\sum_{i>j}\frac{Z_iZ_j}{2m_im_j}\left(\frac{\mathbf{p}_i\mathbf{p}_j}{r_{ij}} + \frac{\mathbf{r}_{ij}(\mathbf{r}_{ij}\mathbf{p}_i)\mathbf{p}_j}{r_{ij}^3}\right) - \frac{e^2}{c^2}\sum_{i>j}4\pi\delta(\mathbf{r}_{ij})Z_iZ_j\left(\frac{c_D^{(i)}}{8m_i^2} + \frac{c_D^{(j)}}{8m_j^2}\right)$$
$$-\frac{e^2}{c^2}\sum_{j\neq i}\frac{Z_iZ_jc_S^{(j)}[\mathbf{r}_{ij}\times\mathbf{p}_j]\mathbf{s}_j}{2m_j^2r_{ij}^3} - \frac{e^2}{c^2}\sum_{i>j}\frac{Z_iZ_j\left(c_F^{(i)}[\mathbf{r}_{ij}\times\mathbf{p}_j]\mathbf{s}_i - c_F^{(j)}[\mathbf{r}_{ij}\times\mathbf{p}_i]\mathbf{s}_j\right)}{m_im_jr_{ij}^3}$$
$$+\sum_{i>j}\left\{\left[\frac{\boldsymbol{\mu}_i\boldsymbol{\mu}_j}{r_{ij}^3} - 3\frac{(\boldsymbol{\mu}_i\mathbf{r}_{ij})(\boldsymbol{\mu}_j\mathbf{r}_{ij})}{r_{ij}^5}\right] - \frac{8\pi}{3}\boldsymbol{\mu}_i\boldsymbol{\mu}_j\delta(\mathbf{r}_{ij})\right\}.$$

Here $\boldsymbol{\mu}_i = c_F^{(i)}Z_i(e\hbar/2m_ic)\,\boldsymbol{\sigma}_i$ is an operator of magnetic moment of a particle.

Self-energy correction in the NRQED. Low energy.

$$k < \Lambda$$



The ultrasoft scale contribution may be expressed:

$$E_L = \frac{2\alpha}{3\pi m^2} \int_0^\Lambda k\,dk \left\langle \mathbf{p} \left(\frac{1}{E_0 - H - k} \right) \mathbf{p} \right\rangle - \delta m \, \langle \psi_0 | \psi_0 \rangle .$$

The integrand may be further rearranged using the operator identity

$$(E_0 - H - k)^{-1} = -1/k - \frac{1}{k^2}(E_0 - H) + \frac{1}{k^2} \frac{(E_0 - H)^2}{E_0 - H - k}$$

that results in

$$E_L = \frac{2\alpha}{3\pi m^2} \left[-\langle \mathbf{p}^2 \rangle \Lambda + \langle \mathbf{p}\,[H, \mathbf{p}] \rangle \ln \Lambda + \int \frac{dk}{k} \left\langle \mathbf{p} \frac{(E_0 - H)^2}{E_0 - H - k} \mathbf{p} \right\rangle \right]$$
$$-\delta m \, \langle \psi_0 | \psi_0 \rangle .$$

Self-energy correction in the NRQED. High energy.

Let us consider the Darwin term in the NRQED Lagrangian

$$\boxed{c_D \frac{e}{8m^2}\left[\mathbf{DE}\right]}$$

For an electron the coefficients c_D is defined as follows

$$c_D = 1 + 2a_e + \frac{\alpha}{\pi}\frac{8}{3}\left[\ln\left(\frac{m}{2\Lambda}\right) + \frac{5}{6} - \frac{3}{8}\right] + \dots$$

where a_e is the anomalous magnetic moment of an electron, Λ is a NRQED cutoff parameter.

Self-energy correction in the NRQED. High energy.

Here we take the $m\alpha^5$ order contribution from the NRQED Lagrangian Darwin term:

$$E_H = -\frac{c_D^{(5)}}{8m^2} 4\pi Z\alpha\langle\delta(\mathbf{r})\rangle, \qquad c_D^{(5)} = 2\frac{\alpha}{2\pi} + \frac{\alpha}{\pi}\frac{8}{3}\left[\ln\left(\frac{m}{2\Lambda}\right) + \frac{5}{6} - \frac{3}{8}\right].$$

Then we get for the self-energy contribution for S states

$$E_H = \frac{\alpha}{3\pi m^2}\left[\ln\alpha^{-2} + \ln\frac{E_h}{\Lambda} - \ln 2 + \frac{5}{6}\right] 4\pi Z\alpha\langle\delta(\mathbf{r})\rangle.$$

Summing up the E_L and E_H contributions we see that the cutoff parameter Λ cancels out and we've got a finite expression for the self-energy contribution.

Self-energy correction for a bound state

Replacing $E_h \to 2R_\infty$, we arrive at the well-known expression[1]

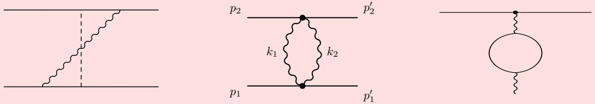
$$\Delta E_{se} = \frac{4\alpha(Z\alpha)}{3m^2}\left[\ln\alpha^{-2} - \ln[k_0(n,l)/R_\infty] + \frac{5}{6}\right]\langle\psi|\delta(\mathbf{r})|\psi\rangle + \frac{\alpha(Z\alpha)}{2\pi m^2}\left\langle\psi\left|\frac{\mathbf{r}\times\mathbf{p}}{r^3}\cdot\frac{\boldsymbol{\sigma}}{2}\right|\psi\right\rangle.$$

where $\ln(k_0/R_\infty)$ is the Bethe logarithm

$$\ln\left[k_0(n,l)/R_\infty\right] = \sum_n \frac{\mathbf{p}_{0n}\mathbf{p}_{n0}(E_n-E_0)\ln(|E_n-E_0|/R_\infty)}{\mathbf{p}_{0n}\mathbf{p}_{n0}(E_n-E_0)},$$

[1] H.A. Bethe and E.E. Salpeter, *Quantum mechanics of one– and two–electron atoms*, Plenum Publishing Co., New York, 1977.

Leading order radiative corrections. Recoil effects



$$\delta^{(3)}E = \alpha^3\left[\frac{4Z}{3}\left(-\ln\alpha^2-\beta(L,v)+\frac{5}{6}-\frac{1}{5}\right)\langle\delta(\mathbf{r})\rangle \right.$$
$$\left. +\frac{2Z^2}{3M}\left(-\ln\alpha-4\,\beta(L,v)+\frac{31}{3}\right)\langle\delta(\mathbf{r})\rangle-\frac{14Z^2}{3M}Q(r)\right],$$

where

$$\beta(L,v)=\frac{\langle\mathbf{J}(H_0-E_0)\ln\left((H_0-E_0)/R_\infty\right)\mathbf{J}\rangle}{\langle[\mathbf{J},[H_0,\,\mathbf{J}]]/2\rangle}$$

is the Bethe logarithm, $\mathbf{J}=\sum_a z_a\mathbf{p}_a/m_a$ is the electric current density operator of the system, and

$$Q(r)=\lim_{\rho\to 0}\left\langle\frac{\Theta(r-\rho)}{4\pi r^3}+(\ln\rho+\gamma_E)\delta(\mathbf{r})\right\rangle.$$

Higher order corrections.

Electron in an external field

Form factors of an electron

Radiative corrections to the electron scattering in the external field lead to appearance of nontrivial form factors:

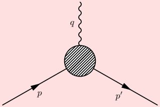
$$F_1(q^2) = 1 - \frac{\mathbf{q}^2}{m^2}\left[\frac{1}{3}\left(\ln\frac{m}{2\Lambda}+\frac{5}{6}-\frac{3}{8}\right)\frac{\alpha}{\pi} - \left(\frac{3}{4}\zeta(3)-\frac{\pi^2}{2}\ln 2+\frac{49\pi^2}{432}+\frac{4819}{5184}\right)\left(\frac{\alpha}{\pi}\right)^2+\dots\right]$$

$$a_e F_2(q^2) = \left[\frac{\alpha}{2\pi}+\left(\frac{3}{4}\zeta(3)-\frac{\pi^2}{2}\ln 2+\frac{\pi^2}{12}+\frac{197}{144}\right)\left(\frac{\alpha}{\pi}\right)^2+\dots\right]-\frac{\alpha}{\pi}\frac{\mathbf{q}^2}{12m^2}+O(q^4),$$

where a_e is the anomalous magnetic moment. "Radiative" form factors determine corrections of orders α, α^2, etc. to "renormalized" constants appeared in NRQED

$$\begin{cases} c_D = 1 + 2a_e + 8m^2 F_1'(0) \\ c_S = 1 + 2a_e, \\ c_F = 1 + a_e. \end{cases}$$

NRQED Lagrangian for the 3-point vertex



$$L_{\rm main} = \psi_e^* \left(-eA_0 + c_F \frac{e}{2m}\boldsymbol{\sigma}\mathbf{B} + c_D \frac{e}{8m^2}\Bigl(\mathbf{D}\mathbf{E}-\mathbf{E}\mathbf{D}\Bigr) + c_S \frac{ie}{8m^2}\,\boldsymbol{\sigma}\cdot\Bigl(\mathbf{D}\times\mathbf{E}-\mathbf{E}\times\mathbf{D}\Bigr)\right)\psi_e$$
$$+\psi_e^*\Biggl(c_W \frac{e}{8m^3}\Bigl\{\mathbf{D}^2,\boldsymbol{\sigma}\mathbf{B}\Bigr\} + c_{q^2}\frac{e}{8m^3}\boldsymbol{\sigma}\cdot[\Delta\mathbf{B}] + c_{p'p}\frac{e}{8m^3}\Bigl\{\mathbf{D}\cdot\mathbf{B}\,\boldsymbol{\sigma}\cdot\mathbf{D}\Bigr\}$$
$$+c_M\frac{ie}{8m^3}\Bigl\{\mathbf{D}\cdot[\mathbf{D}\times\mathbf{B}]+[\mathbf{D}\times\mathbf{B}]\cdot\mathbf{D}\Bigr\}\Biggr)\psi_e$$
$$+\psi_e^*\Biggl(c_{X_1}\frac{e}{128m^4}\Bigl[\mathbf{D}^2,(\mathbf{D}\mathbf{E}+\mathbf{E}\mathbf{D})\Bigr] + c_{X_2}\frac{e}{64m^4}\Bigl\{\mathbf{D}^2,[\boldsymbol{\nabla},\mathbf{E}]\Bigr\} + c_{X_3}\frac{e}{8m^4}\Bigl[\Delta\,[\boldsymbol{\nabla},\mathbf{E}]\Bigr]$$
$$+c_{Y_1}\frac{ie}{64m^4}\Bigl\{\mathbf{D}^2,\boldsymbol{\sigma}\cdot\Bigl(\mathbf{D}\times\mathbf{E}-\mathbf{E}\times\mathbf{D}\Bigr)\Bigr\} + c_{Y_2}\frac{ie}{4m^4}\,\epsilon_{ijk}\sigma^i D^j[\mathbf{D}\mathbf{E}]D^k\Biggr)\psi_e.$$

1. $c_F = 1 + a_e, \qquad c_S = 1 + 2a_e, \qquad c_D = 1+2a_e+\frac{\alpha}{\pi}\frac{8}{3}\left[L-\frac{3}{8}\right],$

2. $c_W = 1, \qquad c_{q^2} = \frac{a_e}{2}+\frac{\alpha}{\pi}\frac{4}{3}\left[L-\frac{3}{8}+\frac{1}{4}\right], \qquad c_{p'p} = a_e,$

$$c_M = -\frac{a_e}{2}-\frac{\alpha}{\pi}\frac{4}{3}\left[L-\frac{3}{8}\right],$$

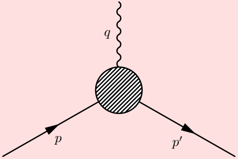
3. $c_{X_1} = 5+4a_e, \qquad c_{X_2} = 3+4a_e, \qquad c_{X_3} = \frac{\alpha}{\pi}\left[\frac{11}{15}L-\frac{59}{120}+\frac{1}{6}\right],$

4. $c_{Y_1} = 3+4a_e, \qquad c_{Y_2} = -\frac{\alpha}{\pi}\frac{1}{3}\left[L-\frac{3}{8}+\frac{1}{2}\right].$

$$\boxed{L = \ln\left(\frac{m}{2\Lambda}\right)+\frac{5}{6}}$$

Complex particles

Form factors of a proton



If a particle of spin 1/2 has internal structure (proton) then the vertex function in the QED for this particle in accordance with requirements of relativistic invariance should has a form

$$\Gamma^{\mu} = \gamma^{\mu} F_1(q^2) + \frac{i\kappa_p}{2m_p}\sigma^{\mu\nu} q_{\nu} F_2(q^2), \qquad F_1(0) = F_2(0) = 1.$$

The NRQED Lagrangian contribution for a proton:

$$\mathcal{L} = -\psi_p^* \left(c_F^{(p)} \frac{e}{2m} \boldsymbol{\sigma}\mathbf{B} + c_D^{(p)} \frac{e}{8m^2} [\mathbf{DE}] + c_S^{(p)} \frac{e}{8m^2} \left\{ \boldsymbol{\sigma} \cdot [i\mathbf{D} \times \mathbf{E}] \right\} \right) \psi_p$$

Arbitrary spin. Spin-orbit interaction.

Leading order spin-orbit interaction for a particle with arbitrary spin $\mathbf{I}$ may be obtained from classical electrodynamics[1]. Since the acceleration of a particle is caused by an electric field $\mathbf{E}$

$$M\frac{d\mathbf{v}}{dt} = Ze\mathbf{E}.$$

To the particle moving with velocity v through this electric field, there will appear to be a magnetic field

$$H_E = \mathbf{E} \times \mathbf{v}/c$$

If this particle has a magnetic moment $\boldsymbol{\mu} = g\mu_N(\mathbf{I}/\hbar)$, it gives an interaction with the field $\mathbf{E}$

$$H_E = -\boldsymbol{\mu} \cdot \mathbf{H}_E = -\boldsymbol{\mu}\left(\mathbf{E} \times \frac{\mathbf{v}}{c}\right),$$

[1] N.F. Ramsey, Phys. Rev. **90**, 232 (1953).

Arbitrary spin. Magnetic moment.

In addition, there will be purely kinematical *Thomas precession*[1]

$$H_T = \hbar\mathbf{I}\,\frac{d\mathbf{v}}{dt}\,\frac{\mathbf{v}}{2c^2} = \hbar\mathbf{I}\,\frac{Ze}{2Mc}\left(\mathbf{E}\times\frac{\mathbf{v}}{c}\right)$$

Summing up, one gets ($\gamma = g\mu_N/\hbar$):

$$\boxed{H_A = -\boldsymbol{\mu}\left[1-\frac{Ze}{2Mc\gamma}\right]\left(\mathbf{E}\times\frac{\mathbf{v}}{c}\right)}$$

[1] L.H. Thomas, Nature (London) **117**, 514 (1926).

Deuteron quadruple moment

An interaction of a *quadruple moment* and a *charge* is derived as follows. Quadruple tensor of a particle of spin s is defined:

$$Q^{ij} = \frac{3Qe}{2s(2s-1)}\left[\left(s^i s^j + s^j s^i\right) - \frac{2s(s+1)}{3}\delta^{ij}\right],$$

it is normalized by the condition,

$$Q^{zz}(m_z) = \frac{Qe}{s(2s-1)}\left[3m_z^2 - s(s+1)\right], \qquad Q^{zz}(s) = Qe.$$

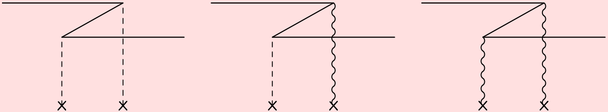
Then, an interaction with a charge is expressed:

$$H_q = Ze^2\frac{Q^{ij}n_in_j}{2r^3} = \frac{Ze^2Q}{2s(2s-1)}\,\frac{3\left(\mathbf{ns}\right)^2 - \mathbf{n}^2\mathbf{s}^2}{r^3}.$$

Higher order corrections

Z-diagrams

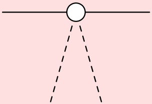
Another kind of contributions for a Dirac electron in an external field, which is related to the order $m\alpha^6$, comes from two-photon exchange diagrams in QED:



$$V_{CC} = -\int \frac{d\mathbf{q}_1}{(2\pi)^3}\int \frac{d\mathbf{q}_2}{(2\pi)^3}\,\frac{4\pi}{q_1^2}\,\frac{4\pi}{q_2^2}(2\pi)^3\delta(\mathbf{q}_1+\mathbf{q}_2-\mathbf{q})\times\frac{u^+(p')\Lambda_-(p+q_1)u(p)}{m+E-E_p-E_{p+q_1}-E_{p'}}$$

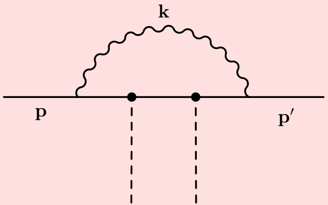
where $\Lambda_-(p)=\frac{E_p-\boldsymbol{\alpha}\mathbf{p}-\beta m}{2E_p}$ is a projection operator on the subspace of states of negative energies.

Relevant contribution that appears in NRQED



$$\frac{e^2}{8m^3}\mathbf{E}^2$$

Self-energy diagram with two Coulomb legs



$$H^{se}_{2\text{-leg}} = \frac{4\pi\alpha(Z\alpha)^2}{m^2}\left(\frac{139}{128} - \frac{1}{2}\ln 2\right)\delta(\mathbf{r})$$

Precision Spectroscopy of HD^+

CODATA18 values and new experiments

The CODATA18 constants:

Rydberg constant	$R_\infty = 10\,973\,731.568\,160(21)\ \mathrm{m}^{-1}$	$1.2\cdot10^{-12}$
deuteron mass	$m_d = 2.013\,553\,212\,745(40)\ \mathrm{u}$	$2.0\cdot10^{-11}$
electron mass	$m_e = 5.485\,799\,090\,65(16)\cdot10^{-4}\ \mathrm{u}$	$2.9\cdot10^{-11}$

Electron-to-proton mass ratio:

	m_p/m_e	m_d/m_p
CODATA18	1836.15267343(11)	1.99900750139(10)
Blaum[1]	1836.152673358(55)	1.999007501228(59)
Myers[2]	1836.152673535(55)	1.999007501274(38)

[1]) S. Rau *et al.* Nature **585**, 43 (2020).
[2]) D.J. Fink, E.G. Myers. Phys. Rev. Lett. **124**, 013001 (2020).

HD^+. Theory and experiment

Theoretical and experimental spin-averaged transition frequencies (in kHz). CODATA18 values of fundamental constants were used in the calculations.

$(L,v) \to (L',v')$	theory	experiment
$(0,0) \to (1,0)$	1 314 925 752.932(19)	1 314 925 752.910(17)
$(0,0) \to (1,1)$	58 605 052 163.9(0.5)	58 605 052 164.24(86)
$(3,0) \to (3,9)$	415 264 925 502.8(3.3)	415 264 925 501.8(1.3)

Results

Reduced mass $\mu = \dfrac{m_p m_d}{(m_p+m_d)m_e}$ inferred from the HD^+ ion spectroscopy

	μ
CODATA18	$1223.899\,228\,722(51)$
$(0,0)\to(0,1)$	$1223.899\,228\,743(16)_{exp}(17)_{th}$
$(0,0)\to(1,1)$	$1223.899\,228\,707(17)_{exp}(17)_{th}$
$(3,0)\to(3,9)$	$1223.899\,228\,730(04)_{exp}(17)_{th}$
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Relative uncertainty: $u_r(\mu) = 1.4\times10^{-11}$.

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Mass ratios from spectroscopy and Myers' experiment:

$$m_p/m_e = 1836.152673476(44), \qquad m_d/m_e = 3670.482967763(88),$$

Thank you for your attention!