Towards a bound-state relativistic QED approach

Dávid Ferenc

ELTE
Molecular Quantum Dynamics Research Group

25 May 2023

Introduction

Motivation

- Theoretical description high-precision spectroscopy measurements
- Light, few-particle bound states (H, Ps, Mu, He, H_2^+, H_2, He_2^+,...)

We need a relativistic bound-state QED approach

Bound state QED

$$\mathcal{L} = -\frac{1}{4}F_{\mu\nu}F^{\mu\nu} + \bar{\psi}\left(\mathrm{i}\gamma^{\mu}\partial_{\mu} - m\right)\psi - e\bar{\psi}\gamma^{\mu}\psi A_{\mu}$$

‘textbook’ QED

- Perturbation expansion around non-interacting fields
- For S matrix: only few photons
- For bound states: arbitrary number of photons

Nonrelativistic QED (NRQED)

- Expand solutions of Dirac equation in $Z\alpha$
- Calculate every interaction up to a given order in α
- Main challenge: derivation of higher order terms (necessary for high precision experiments)

Bethe–Salpeter approach

- Avoid nonrelativistic expansion
- Account for particle-particle interaction & external field in zeroth order

Bethe–Salpeter approach

- Avoid nonrelativistic expansion
- Account for particle-particle interaction & external field in zeroth order

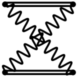
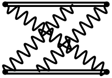
The Bethe–Salpeter equation

$$\varphi(x_1,x_2) = -\mathrm{i}\int \mathrm{d}^4x_3\mathrm{d}^4x_4\mathrm{d}^4x_5\mathrm{d}^4x_6\; S_1(x_1,x_5)S_2(x_2,x_6)K(x_5,x_6;x_3,x_4)\varphi(x_3,x_4)$$

- $S(x,x')$ (external-field) fermion propagator

$$(\mathrm{i}\partial_{t_1} - h_1)\, S_1(x,x') = \mathrm{i}\beta_1\delta(x-x') \qquad h_1 = \boldsymbol{\alpha}_1\cdot\boldsymbol{p}_1 + m_1\beta_1 + V_{\mathrm{nuc}}(\boldsymbol{r}_1)$$

- $K(x_1,x_2;x_1',x_2')$ irreducible interaction kernel

$K =$  $+$  $+$  $+\ \dots$

Salpeter, Bethe, Phys. Rev. 84, 1232 (1951)

Bethe–Salpeter approach

- Introduce absolute- and relative time, and the ansatz

$$T = \frac{1}{2}(t_1 + t_2) \qquad t = t_1 - t_2 \qquad \varphi(x_1, x_2) = \mathrm{e}^{-\mathrm{i}ET}\phi(\boldsymbol{r}_1, \boldsymbol{r}_2, t)$$

- In momentum space after rearrangement

$$\mathcal{F}\psi(\boldsymbol{p}_1, \boldsymbol{p}_2, \varepsilon) = \mathcal{K}\psi(\boldsymbol{p}_1, \boldsymbol{p}_2, \varepsilon)$$

$$\mathcal{K} = \mathcal{K}_\mathrm{i} + \mathcal{K}_\Delta$$

  - $\mathcal{K}_\mathrm{i}$ is chosen to be instantaneous (e.g.: Coulomb or Coulomb–Breit)

$$\begin{aligned}\mathcal{K}_\mathrm{i} f(\boldsymbol{p}_1, \boldsymbol{p}_2, \varepsilon) &= (-2\pi\mathrm{i})^{-1} \int \mathrm{d}\boldsymbol{k}\, \mathrm{d}\omega\, \kappa_\mathrm{i}(\boldsymbol{k}) f(\boldsymbol{p}_1 - \boldsymbol{k}, \boldsymbol{p}_2 + \boldsymbol{k}, \varepsilon - \omega) \\ &= (-2\pi\mathrm{i})^{-1} \int \mathrm{d}\omega\, \mathcal{I}_\mathrm{i} f(\boldsymbol{p}_1, \boldsymbol{p}_2, \varepsilon - \omega)\end{aligned}$$

Salpeter, Phys. Rev. 87, 328 (1952), Sucher, PhD thesis (1958)
Mátyus, Ferenc, Jeszenszki, Margócsy, ACS Phys. Chem. Au (2023)

Exact equal-time approach

The equal-time equaiton

$$\Psi(\boldsymbol{p}_1, \boldsymbol{p}_2) = \int \mathrm{d}\varepsilon \; \psi(\boldsymbol{p}_1, \boldsymbol{p}_2, \varepsilon)$$

$$\Psi(\boldsymbol{p}_1, \boldsymbol{p}_2) = \int \frac{\mathrm{d}\varepsilon}{-2\pi\mathrm{i}} \; \mathcal{F}^{-1} \mathcal{I}_{\mathrm{i}} \Psi(\boldsymbol{p}_1, \boldsymbol{p}_2) + \int \frac{\mathrm{d}\varepsilon}{-2\pi\mathrm{i}} \; \mathcal{F}^{-1} \mathcal{K}_\Delta \left(\mathcal{F} - \mathcal{K}_\Delta\right)^{-1} \mathcal{I}_{\mathrm{i}} \Psi(\boldsymbol{p}_1, \boldsymbol{p}_2)$$

$$\begin{aligned} \int \frac{\mathrm{d}\varepsilon}{-2\pi\mathrm{i}} \mathcal{F}^{-1} &= \int \frac{\mathrm{d}\varepsilon}{-2\pi\mathrm{i}} \left(E/2 - \varepsilon - h_2\right)^{-1} \left(E/2 + \varepsilon - h_1\right)^{-1} \\ &= \left(E - h_1 - h_2\right)^{-1} \big(\underbrace{\Lambda_+ \Lambda_+}_{\Lambda_{++}} - \underbrace{\Lambda_- \Lambda_-}_{\Lambda_{--}}\big) \end{aligned}$$

Salpeter, Phys. Rev. 87, 328 (1952), Sucher, PhD thesis (1958)
Mátyus, Ferenc, Jeszenszki, Margócsy, ACS Phys. Chem. Au (2023)

The exact equal-time equation

$$(H + H_\Delta)\Psi(\boldsymbol{r}_1, \boldsymbol{r}_2) = E\Psi(\boldsymbol{r}_1, \boldsymbol{r}_2) \qquad H = h_1 + h_2 + \Lambda_{++}\mathcal{I}_\mathrm{i}\Lambda_{++}$$

$$\begin{aligned} H_\Delta =& \Lambda_{++}\mathcal{I}_\mathrm{i}(1 - \Lambda_{++}) - \Lambda_{--}\mathcal{I}_\mathrm{i} \\ &+ (E - h_1 - h_2)^{-1} \int \frac{\mathrm{d}\varepsilon}{-2\pi\mathrm{i}} \mathcal{F}^{-1}\mathcal{K}_\Delta(\mathcal{F} - \mathcal{K}_\Delta)^{-1}\mathcal{I}_\mathrm{i} \end{aligned}$$

$$\mathcal{F}^{-1}\mathcal{K}_\Delta(\mathcal{F} - \mathcal{K}_\Delta)^{-1} = \mathcal{F}^{-1}\mathcal{K}_\Delta\mathcal{F}^{-1} + \mathcal{F}^{-1}\mathcal{K}_\Delta\mathcal{F}^{-1}\mathcal{K}_\Delta\mathcal{F}^{-1} + \ldots$$

- H: no-pair Dirac–Coulomb(–Breit) Hamiltonian
- Retardation, pair- and radiative corrections in H_Δ
- Perturbative treatment of terms in H_Δ seems possible
- *High-precision variational zeroth order solution is possible*

Mátyus, Ferenc, Jeszenszki, Margócsy, ACS Phys. Chem. Au (2023)

The no-pair Dirac–Coulomb(–Breit) equation

The Hamiltonian

$$H(1,2) =$$
$$\Lambda_{++}\begin{pmatrix} V1^{[4]} + U1^{[4]} & c\boldsymbol{\sigma}_2^{[4]}\cdot\boldsymbol{p}_2 & c\boldsymbol{\sigma}_1^{[4]}\cdot\boldsymbol{p}_1 & B^{[4]} \\ c\boldsymbol{\sigma}_2^{[4]}\cdot\boldsymbol{p}_2 & V1^{[4]} + (U-2m_2c^2)1^{[4]} & B^{[4]} & c\boldsymbol{\sigma}_1^{[4]}\cdot\boldsymbol{p}_1 \\ c\boldsymbol{\sigma}_1^{[4]}\cdot\boldsymbol{p}_1 & B^{[4]} & V1^{[4]} + (U-2m_1c^2)1^{[4]} & c\boldsymbol{\sigma}_2^{[4]}\cdot\boldsymbol{p}_2 \\ B^{[4]} & c\boldsymbol{\sigma}_1^{[4]}\cdot\boldsymbol{p}_1 & c\boldsymbol{\sigma}_2^{[4]}\cdot\boldsymbol{p}_2 & V1^{[4]} + (U-2m_{12}c^2)1^{[4]} \end{pmatrix}\Lambda_{++}$$

Restricted kinetic balance

$$\psi^{\text{s}} \approx \frac{\boldsymbol{\sigma}^{[2]}\cdot\boldsymbol{p}}{2mc}\psi^{\text{l}} \qquad \Psi(\boldsymbol{r}_1,\boldsymbol{r}_2) = \begin{pmatrix} \psi^{\text{ll}}(\boldsymbol{r}_1,\boldsymbol{r}_2) \\ \psi^{\text{ls}}(\boldsymbol{r}_1,\boldsymbol{r}_2) \\ \psi^{\text{sl}}(\boldsymbol{r}_1,\boldsymbol{r}_2) \\ \psi^{\text{ss}}(\boldsymbol{r}_1,\boldsymbol{r}_2) \end{pmatrix}$$

$$H_{\text{KB}} = X^{\dagger}HX \qquad I_{\text{KB}} = X^{\dagger}IX$$

$$X = \text{diag}\left(1^{[4]}, -\frac{\left(\boldsymbol{\sigma}_2^{[4]}\cdot\boldsymbol{p}\right)}{2m_2c}, \frac{\left(\boldsymbol{\sigma}_1^{[4]}\cdot\boldsymbol{p}\right)}{2m_1c}, -\frac{\left(\boldsymbol{\sigma}_1^{[4]}\cdot\boldsymbol{p}\right)\left(\boldsymbol{\sigma}_2^{[4]}\cdot\boldsymbol{p}\right)}{4m_1m_2c^2}\right)$$

Two-electron systems in external field

Direct comparison with corresponding NRQED terms

	$E_{\mathrm{DC}}^{++}/E_\mathrm{h}$	$\delta_{\mathrm{DC}}^{(2)}/\mathrm{n}E_\mathrm{h}$	$\delta_{\mathrm{DC}}^{(3)}/\mathrm{n}E_\mathrm{h}$	$\alpha^4\varepsilon_4^*/\mathrm{n}E_\mathrm{h}$
H_2	−1.174 489 754	−21	0	−0.2
H_3^+	−1.343 850 527	−24	−1	
H^-	−0.527 756 733	−3	0	
He (2S)	2.146 084 791	−22	−11	−10.4
He (1S)	−2.903 856 631	−145	−11	−11.2
Li^+	−7.280 698 899	−835	−164	
Be^{2+}	−13.658 257 603	−2952	−1036	

ε_4^*: complete, non-radiative fourth order (after cancellation of divergences with other QED terms) (PRL 117, 263002 (2016), PRA 74, 022512 (2006))

Jeszenszki, Ferenc, Mátyus, JCP 156, 084111 (2022)

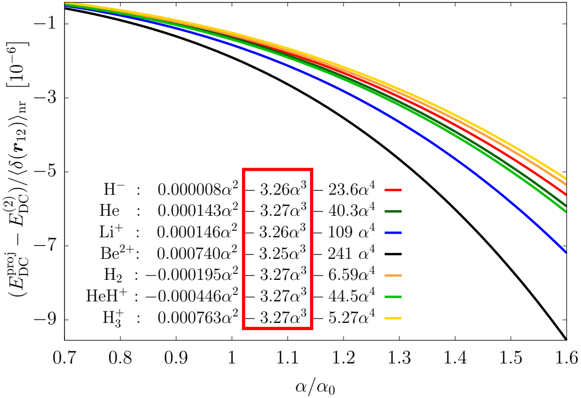
Ferenc, Jeszenszki, Mátyus, JCP 157, 094113 (2022)

Comparison to NRQED

‘α-scaling’

$$E_{\mathrm{DC(B)}}(\alpha) = \epsilon_0 + \alpha^2\epsilon_2 + \alpha^3\epsilon_3 + \alpha^4\ln(\alpha)\epsilon_4' + \alpha^4\epsilon_4$$

Two-electron systems



$$\epsilon_{\mathrm{CC}}^{++} = -\left(\frac{\pi}{2} + \frac{5}{3}\right)\langle\delta(\boldsymbol{r}_{12})\rangle$$
$$\approx -3.24\langle\delta(\boldsymbol{r}_{12})\rangle$$

$$\epsilon_3^{\mathrm{fit}} = -3.26(2)\langle\delta(\boldsymbol{r}_{12})\rangle$$

Comparison to NRQED

'α-scaling'

$$E_{\mathrm{DC(B)}}(\alpha) = \epsilon_0 + \alpha^2\epsilon_2 + \alpha^3\epsilon_3 + \alpha^4\ln(\alpha)\epsilon_4' + \alpha^4\epsilon_4$$

Two-fermion systems: Ps, Mu, H, μH

$$\Psi(\boldsymbol{r}) = \sum_{i=1}^{50}\sum_{\chi=1}^{16} c_{i\chi}\boldsymbol{d}_\chi f_i(\boldsymbol{r}) \qquad f_i(\boldsymbol{r}) = \mathrm{e}^{-\zeta_i r^2}$$

	DC			
	ϵ_0	ϵ_2	ϵ_3	ϵ_4'
$\mathrm{Ps} = \{\mathrm{e}^+, \mathrm{e}^-\}$:				
var-fit	$-0.250\,000\,000\,000$	$0.046\,875$	$-0.128\,8$	$-0.063\,4$
nrQED	$-0.250\,000\,000\,000$	$0.046\,875$	$-0.128\,8$	$-0.062\,5$
$\alpha^n(\delta\varepsilon_n)$	$-3.0\cdot10^{-13}$	$-4.5\cdot10^{-12}$	$7.2\cdot10^{-12}$	$2.6\cdot10^{-12}$

(See also: P-Mo-7) Ferenc, Mátyus, PRA, 107, 052803 (2023)

Current status & challenges

Included in zeroth order

- Exact inclusion of dominant instantaneous photon exchange diagrams
- All-orders in external field

Perturbative

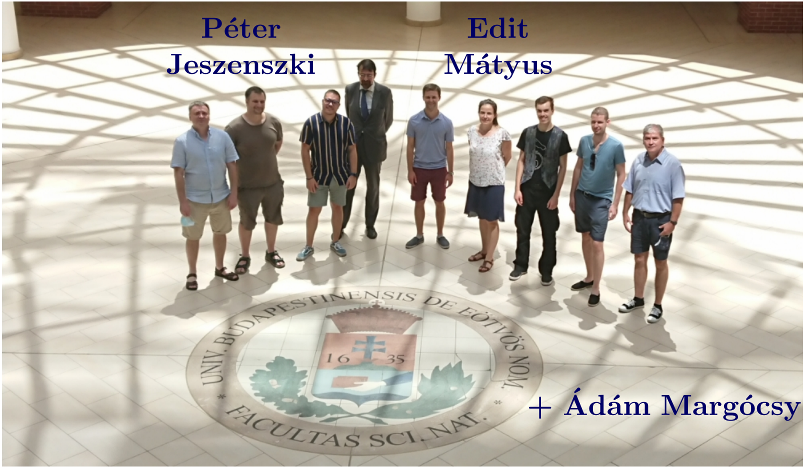
- Pair corrections
- Retardation
- Radiative QED

Work in progress

Summary

- Numerical, high precision no-pair relativistic approach with prospect for including further corrections for QED
- Zeroth order equation is solvable numerically to high precision
- Some of the higher order NRQED terms obtained 'for free'
- 'alpha-scaling' provides an order-by-order test with respect to the corresponding high-precision NRQED corrections
- Perturbative radiative, retardation and pair corrections (in progress)

Jeszenszki, Ferenc, Mátyus, JCP 154, 224110 (2021)
Jeszenszki, Ferenc, Mátyus, JCP 156, 084111 (2022)
Ferenc, Jeszenszki, Mátyus, JCP 156, 084110 (2022)
Ferenc, Jeszenszki, Mátyus, JCP 157, 094113 (2022)
Mátyus, Ferenc, Jeszenszki, Margócsy, ACS Phys. Chem. Au (2023)
Ferenc, Mátyus, PRA, 107, 052803 (2023)



Thank you for your attention!