QED effects in many-electron ions

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Outline

QED in high-Z many-electron ions

– external-field approximation
– bound-state QED bound-state theory
– no-virtual-pair approximation
  (relativistic many-body perturbation theory, RMBPT, RCC, etc.)
– retardation and negative-energy effects
– self-energy and vacuum polarization: renormalization
– many-body corrections to self-energy and vacuum polarization
– one-valence systems: Li-like, Na-like, and Cu-like isoelectronic series
– two-valence systems: Zn-like isoelectronic series
– Outlook: effective-interaction approach in RMBPT calculations
External-field approximation

• Assume nucleus is a stationary source of a classical potential $V_{\text{nuc}}(\mathbf{r})$

Lagrangian of QED:

$$L_{\text{QED}} = \overline{\psi}(i\gamma^\mu \gamma_\mu + \gamma_0 V_{\text{nuc}} - m)\psi + e\overline{\psi}(\gamma_\mu A^\mu)\psi$$

$\psi$ electron field
$A^\mu$ photon field

• Nuclear recoil
  – nonrelativistic, added perturbatively

$$\frac{P_{\text{nuc}}^2}{2M_{\text{nuc}}} \rightarrow \frac{1}{2M_{\text{nuc}}} \left( -\sum_{i=1}^N \mathbf{p}_i \right)^2 = \sum_{i=1}^N \frac{\mathbf{p}_i^2}{2M_{\text{nuc}}} + \sum_{i>j} \frac{\mathbf{p}_i \cdot \mathbf{p}_j}{M_{\text{nuc}}}$$

  – higher-order terms from Bethe-Salpeter equation

• Nuclear finite size: $V_{\text{nuc}}(\mathbf{r})$ generated from Fermi distribution with $\left\langle R^2 \right\rangle_{\text{expt}}$
Bound-state QED perturbation theory

- Partition problem into a zeroth-order part plus an interaction

\[ L_{\text{QED}} = \overline{\psi} \left( i \partial^\mu \gamma_\mu + \gamma_0 V_{\text{nuc}} + \gamma_0 U - m \right) \psi + \overline{\psi} \left( e \gamma_\mu A^\mu - \gamma_0 U \right) \psi \]

\[ L_0 \quad \text{and} \quad L_{\text{int}} \]

\( U \) suitable mean field

- Spectrum of Dirac equation

\[ \psi(r, t) = \sum_{i > 0} \phi_i(r) e^{-iE_i t} a_i + \sum_{i < 0} \phi_i^*(r) e^{iE_i t} b_i^* \]

Numerical basis set (B-splines)

Johnson, Blundell, Sapirstein (1988)
QED perturbation theory

- Diagrammatic expansion:
  - adiabatic S-matrix (Gell-Mann and Low, 1950s)
  - poles in $N$-particle Green’s function (Kato perturbation theory)

- Feynman diagrams:

- Electron propagator
  \[ G(\varepsilon; \mathbf{r}_2, \mathbf{r}_1) = \sum_i \frac{\phi_i(\mathbf{r}_2)\bar{\phi}_i(\mathbf{r}_1)}{\varepsilon - \varepsilon_i \pm i0^+} \]

- Photon interaction
  (frequency dependent)
  \[ \langle ab\mid(\alpha_\mu)_{1}(\alpha_\nu)_{2}D^{\mu\nu}(\omega;12)\mid cd \rangle \]

- Loop integrals
  \[ E_{SE} = i\int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \sum_i \frac{\langle vi\mid(\alpha_\mu)_{1}(\alpha_\nu)_{2}D^{\mu\nu}(\omega;12)\mid iv \rangle}{\varepsilon_v + \omega - \varepsilon_i \pm i0^+} \]
No-virtual-pair (RMBPT) approximation

- Instantaneous photon interactions

\[ \langle ab | \tilde{r}_{12}^{-1} | cd \rangle \]

\[ \langle ab | r_{12}^{-1} \left[ \alpha_1 \cdot \alpha_2 - \frac{1}{2} \left( \alpha_1 \cdot \hat{r}_{12} \right) \left( \alpha_2 \cdot \hat{r}_{12} \right) \right] | cd \rangle \]

- Omit negative-energy states from electron propagators

⇒ An approximate evaluation of a subset of QED perturbation-theory diagrams (RMBPT)
Box diagram

\[ E_{\text{BOX}} = i \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \sum_{c} \sum_{ij \neq vc} \frac{\langle vc | (\alpha_\mu)_1(\alpha_\nu)_2 D^{\mu\nu}(\omega;12)|ij\rangle \langle ij | (\alpha_\mu)_1(\alpha_\nu)_2 D^{\mu\nu}(\omega;12)|vc\rangle}{(\varepsilon_v + \omega - \varepsilon_i \pm i0^+)(\varepsilon_c - \omega - \varepsilon_j \pm i0^+)} \]

- In the RMBPT approximation, this diagram corresponds to

\[ E = \frac{1}{2} \sum_{c,s} \frac{\langle vc|r\rangle \langle rs|vc\rangle}{\epsilon_c + \epsilon_v - \epsilon_r - \epsilon_s} \]

- Allowing \( r \) and \( s \) to extend over negative energy states produces zero denominators
  “Continuum dissolution”
RMBPT and field-theoretic effects

- Self-energy
- Vacuum polarization

Purely field-theoretic
Can regard the RMBPT approximation to QED perturbation theory as being generated via traditional nonrelativistic many-body methods from the Dirac-Coulomb-Breit Hamiltonian

\[ H_{DCB} = \sum_{i=1}^{N} [\alpha_i \cdot p_i + \beta_i mc^2 + V_{\text{nuc}}(r_i)] + \sum_{i \neq j}^{N} \Lambda_{++} \left( \frac{e^2}{r_{ij}} + B_{ij} \right) \Lambda_{++} \]

positive-energy projection operators

RMBPT
- Li-like isoelectronic series Johnson, Blundell, Sapirstein (1987)
- Na-like (1988)
- Cu-like (1990)

RCC
- Cs parity nonconserving amplitude (FS-LCCSDvT\textsubscript{S}-3) Blundell, Johnson, Sapirstein (1990)
Retardation: single photon exchange

- Consider one valence electron outside a closed-shell core

\[ B_{v}^{(1)} = - \sum_{c} \langle vc | b_{12} | cv \rangle \]

\[ E_{1\text{-photon}} = - \sum_{c} \langle vc | (\alpha_{\mu})_{1} (\alpha_{v})_{2} D^{uv} \left( \epsilon_{v} - \epsilon_{c}; 12 \right) | cv \rangle \]

e.g., Cu-like ions: \( Z = 92 \) (atomic units)

<table>
<thead>
<tr>
<th></th>
<th>( B^{(1)} )</th>
<th>Ret.(^{(1)} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>( 4s-4p_{1/2} )</td>
<td>0.1008</td>
<td>0.0027</td>
</tr>
<tr>
<td>( 4s-4p_{3/2} )</td>
<td>-0.0140</td>
<td>-0.0195</td>
</tr>
<tr>
<td>( 4s-4d_{3/2} )</td>
<td>-0.0480</td>
<td>-0.0019</td>
</tr>
<tr>
<td>( 4s-4d_{5/2} )</td>
<td>-0.0921</td>
<td>-0.0038</td>
</tr>
</tbody>
</table>

\[ Z(Z \alpha)^{2} \quad Z(Z \alpha)^{4} \]
Self-energy and vacuum polarization: renormalization

• Both the self-energy and the vacuum polarization are *ultra-violet divergent*

  – part of the self-energy corresponds to modifying the mass of the electron
    ⇒ effective term $\delta m \overline{\psi} \psi$ in the Lagrangian

  – since we use the experimentally measured mass, we must subtract this piece

  – the divergence is subtracted in the process

  self-energy

  – part of the vacuum polarization corresponds to modifying the electric charge
    $$e \rightarrow e + \delta e$$

  – divergence is associated entirely with $\delta e$

  – all divergences in QED are associated either with $\delta e$ or $\delta m$
    ⇒ theory becomes finite

  vacuum polarization
Renormalization: potential expansions

- Expand electron propagator in terms of external potential

\[
\text{bound propagator} = \text{free propagator} + \text{X} + \text{X} + \text{X} + \ldots
\]

\[V_{\text{ext}} = V_{\text{nuc}} + U\]

- Subtraction made analytically (momentum-space integrals)

- Many-potential term

S. A. Blundell and N. J. Snyderman (1991) [ Earlier work: Desiderio and Johnson (1971); Mohr (1974/5) ]
Vacuum polarization

\[ \text{Vacuum polarization} = \text{Uehling term (1935)} \text{ (divergent)} + \text{Wichmann-Kroll terms} \text{ (finite)} + \ldots \]
Application to high-\(Z\) ions: \(1/Z\) expansion

- Each order of perturbation theory contributes a factor \(1/Z\)

\[
\frac{\langle ab\|cd\rangle}{\Delta \varepsilon} \sim \frac{Z}{Z^2} = \frac{1}{Z}
\]

- Neutral atoms: all-order methods (RCC)
- High-\(Z\) ions: order-by-order RMBPT/QED-PT

<table>
<thead>
<tr>
<th>Z dependence</th>
<th>atomic units</th>
</tr>
</thead>
<tbody>
<tr>
<td>DF energy</td>
<td>(Z^2)</td>
</tr>
<tr>
<td>Coulomb correlation (E^{(2)})</td>
<td>1</td>
</tr>
<tr>
<td>3rd order Coulomb (E^{(3)})</td>
<td>(1/Z)</td>
</tr>
<tr>
<td>Breit interaction (B^{(1)})</td>
<td>(Z^3)</td>
</tr>
<tr>
<td>Breit-Coulomb (B^{(2)})</td>
<td>(Z^2)</td>
</tr>
<tr>
<td>Retardation (1-photon)</td>
<td>(Z^5)</td>
</tr>
<tr>
<td>Self-energy or vacuum polarization</td>
<td>(Z^4)</td>
</tr>
<tr>
<td>Screening corrections to self-energy</td>
<td>(Z^3)</td>
</tr>
</tbody>
</table>
Zn-like and Cu-like ions

- 28-electron closed-shell Ni-like core: $1s^22s^22p^63s^23p^63d^{10}$

- **Cu-like**: single valence electron

- **Zn-like**: two valence electrons

- Perturbative expansion around Dirac-Fock or Breit-Dirac-Fock potential of the Ni-like core

- Recent experiments (2004) by Beiersdorfer and co-workers

- Relativistic many-body perturbation theory (RMBPT) for Cu-like ions
  
  W. R. Johnson, S. A. Blundell, and J. Sapirstein, PRA 42, 1087 (1990)

  Coulomb correlation through 3rd order, Breit correlation through 2nd order
Many-electron QED effects in Cu-like ions

- 28-electron Ni-like core “screens” self-energy and vacuum polarization, \( Z \rightarrow Z_{\text{eff}} = Z - c \)

- If mean-field potential \( U \) is not \textbf{local}, \( U = U(r) \), self-energy is not finite in lowest-order PT

\[
V = V_{\text{nuc}} + V_{\text{DF,dir}}
\]

- Example, Cu-like Bi (\( Z = 83 \)):

\[\text{SE(screened)} \approx 0.6 \text{ SE(hydrogenic)}\]

Screened self-energy and vacuum polarization

- Direct screening diagrams accounted for to all orders by including $V_{DF,dir}$ in electron propagators
- Canceled by $-U$ in residual interaction
Smaller screening effects

- Valence-core exchange interaction

- Neglect vertex correction and photon self-energy diagram

- Example, Cu-like Bi ($Z = 83$) 4s state:
  \[
  \text{SE(dir.)} \sim 0.6 \text{SE(hyd)} \\
  \text{SE(exch.)} \sim 0.01 \text{SE(hyd)}
  \]

- Screening by **direct** part of potential \( \sim \frac{N_{\text{core}}}{Z} \text{SE(hyd)} \)
  exchange part of potential \( \sim \frac{1}{Z} \text{SE(hyd)} \)

- Core relaxation
### Cu-like U (U^{63+})

Units: eV

<table>
<thead>
<tr>
<th></th>
<th>$4s-4p_{3/2}$</th>
<th>$4p_{1/2}-4d_{3/2}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>RMBPT-3</td>
<td>472.280</td>
<td>535.690</td>
</tr>
<tr>
<td>SE (valence)</td>
<td>$-4.226(2)$</td>
<td>$-0.843(2)$</td>
</tr>
<tr>
<td>VP (valence)</td>
<td>1.165(5)</td>
<td>0.214(2)</td>
</tr>
<tr>
<td>Exchange (SE+VP)</td>
<td>0.048</td>
<td>0.010</td>
</tr>
<tr>
<td>Core (SE+VP)</td>
<td>$-0.042$</td>
<td>0.047</td>
</tr>
<tr>
<td>Theory</td>
<td>469.23</td>
<td>535.12</td>
</tr>
<tr>
<td>Expt.</td>
<td>469.22(3)</td>
<td>535.15(5)</td>
</tr>
<tr>
<td>Theory – expt.</td>
<td>0.01(3)</td>
<td>0.03(5)</td>
</tr>
</tbody>
</table>

4s-4p\textsubscript{3/2} transition in Cu-like ions


Zn-like ions: relativistic correlation

- Two valence electrons outside 28-electron closed-shell Ni-like core: $1s^2 2s^2 2p^6 3s^2 3p^6 3d^{10}$

- Valence space: $4s$, $4p_{1/2}$, $4p_{3/2}$, $4d_{3/2}$, $4d_{5/2}$, $4f_{5/2}$, $4f_{7/2}$

- Use a FS-RMBPT

$$H_{\text{eff}} C = E C$$

Effective Hamiltonian \quad energies

e.g. $J = 1$, odd parity: 8 possible states within valence space

$$|4s 4p_{1/2}\rangle_{J=1} \quad |4s 4p_{3/2}\rangle_{J=1} \quad |4p_{1/2} 4d_{3/2}\rangle_{J=1} \quad |4p_{3/2} 4d_{3/2}\rangle_{J=1}$$

$$|4p_{3/2} 4d_{5/2}\rangle_{J=1} \quad |4d_{3/2} 4f_{5/2}\rangle_{J=1} \quad |4d_{5/2} 4f_{5/2}\rangle_{J=1} \quad |4d_{5/2} 4f_{7/2}\rangle_{J=1}$$

- $H_{\text{eff}}$: 8 x 8 matrix (non-symmetric)

  Coulomb and Breit correlation through second order
Many-electron QED effects in Zn-like ions

• Treat self-energy and vacuum polarization terms as effective interactions within RMBPT

• Cu-like QED (SE, VP, valence-core exchange, core relaxation) are one-body effects and enter on diagonal of effective Hamiltonian

\[
\langle v'w' | H_{\text{eff}} | vw \rangle = \delta_{v'v} \delta_{w'w} (\delta \varepsilon_v + \delta \varepsilon_w)
\]

• Valence-valence screening terms

Two-body effects, enter on diagonal and off-diagonal parts of effective Hamiltonian
4s$^2$$^1$S$_0$ – 4s4p $^1$P$_1$ transition in Zn-like ions

Units: eV

<table>
<thead>
<tr>
<th></th>
<th>Th$^{60+}$</th>
<th>U$^{62+}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>RMBPT-2</td>
<td>434.770(2)</td>
<td>477.006(1)</td>
</tr>
<tr>
<td>Retardation</td>
<td>−0.469</td>
<td>−0.529</td>
</tr>
<tr>
<td>SE (valence)</td>
<td>−3.772</td>
<td>−4.201</td>
</tr>
<tr>
<td>VP (valence)</td>
<td>1.000</td>
<td>1.158</td>
</tr>
<tr>
<td>Exchange (SE+VP)</td>
<td>0.044</td>
<td>0.047</td>
</tr>
<tr>
<td>Core (SE+VP)</td>
<td>−0.040</td>
<td>−0.041</td>
</tr>
<tr>
<td>2-body (SE+VP)</td>
<td>0.026(5)</td>
<td>0.028(5)</td>
</tr>
<tr>
<td>2-loop</td>
<td>0.013(5)</td>
<td>0.015(6)</td>
</tr>
<tr>
<td>Theory</td>
<td>431.573</td>
<td>473.483</td>
</tr>
<tr>
<td>Expt.</td>
<td>431.545(17)</td>
<td>473.473(18)</td>
</tr>
<tr>
<td>Theory − expt.</td>
<td>0.027(17)</td>
<td>0.009(18)</td>
</tr>
</tbody>
</table>


4s^2 \, ^1S_0 - 4s4p \, ^1P_1 \, \text{transition in Zn-like ions}

Summary and outlook

• Within the external-field approximation to QED, possible to construct a systematic QED perturbation theory for atomic bound states

• The no-virtual-pair approximation (Dirac-Coulomb-Breit Hamiltonian) is a well-defined approximation to a subset of QED perturbation theory

• Use these precise perturbative calculations as a “laboratory” to construct, and test the accuracy of effective interactions for the self-energy and vacuum polarization