Energy-dependent Many-Body-Perturbation Theory

with Applications in Quantum-Electrodynamics Problems

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Outline

- Introduction
  - Definition of QED
  - The need for a combined many-body-QED procedure
- Standard time-independent perturbation theory
- Time-dependent perturbation theory
  - S-matrix formulation
  - Covariant evolution-operator formalism
  - Towards exact treatment

    Including electron correlation. Fock space
- Numerical results of QED effects on He-like ions
- Conclusions and Outlook

Definition of QED

- **Quantum-electrodynamics**
  is the quantum theory of the interaction between electrons and the electro-magnetic radiation field
- **The interaction is energy dependent**
  Standard MBPT procedures cannot be used
- **Our goal is to construct**
  a combined Many-Body-QED procedure

Definition of QED

Standard procedures for QED calculations

- **Analytical methods**
  - Expansion of the Bethe-Salpeter eqn in powers in α and $Z\alpha$ (Drake, Pachucki)

Restricted to light elements

- **Numerical methods**
  - S-matrix (Only for single-reference model space. Cannot treat quasidegeneracy
  - Two-times Green's function (Shabaev et al. 1993)
  - Covariant evolution operator (Lindgren et al. 2001)

Restricted to heavy elements

Definition of QED

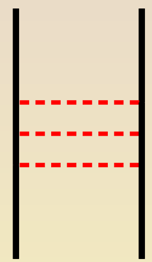
- The exact treatment of a two-electron system requires the solution of the Bethe-Salpeter equation
- Normally based upon the Brillouin-Wigner perturbation theory
- Using the covariant-evolution operator expansion to all orders is equivalent to solving the BS eqn
  Lindgren, Salomonson, and Hedendahl, Can. J. Phys. 83, 183 (2005)
- Gives the link between BS eqn and Many-Body Perturbation Theory (based upon Rayleigh-Schrödinger PT)

Standard Many-Body Procedures

Non-relativistic atomic Hamiltonian:

$$\boldsymbol{H = \sum_{i=1}^{N} h_S(i) + \sum_{i<j}^{N} \frac{1}{r_{ij}} \; ; \qquad h_S = -\frac{1}{2}\nabla^2 - \frac{Z}{r}}$$

- **Many-body perturbation theory** (MBPT)
- **Coupled-Custer Approach** (CCA)
- **Configuration Interaction** (CI)
- **Multi-Configuration Hartree-Fock** (MCHF)



Can treat electron correlation to essentially all orders

Definition of QED

Relativistic Dirac-Coulomb-Breit Hamiltonian

$$H = \Lambda_+ \Big[\sum_{i=1}^{N} h_D(i) + \sum_{i<j}^{N} \frac{1}{r_{ij}} + H_B \Big] \Lambda_+$$

Breit interaction, 1932-33

$$H_B = -\frac{1}{2} \sum_{i<1} \Big[\alpha_i \cdot \alpha_j + \frac{(\alpha_i \cdot r_{ij})(\alpha_j \cdot r_{ij})}{r_{ij}^2} \Big]$$

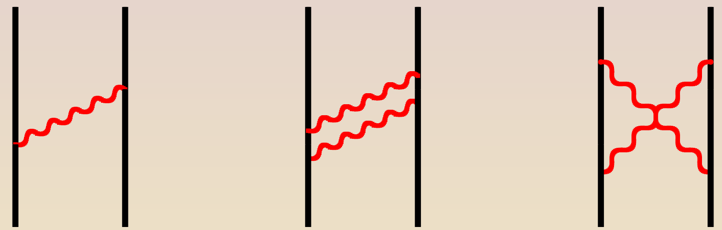
Retardation and virtual pairs neglected

No-virtual-pair approximation (NVPA)

(Sucher 1980)

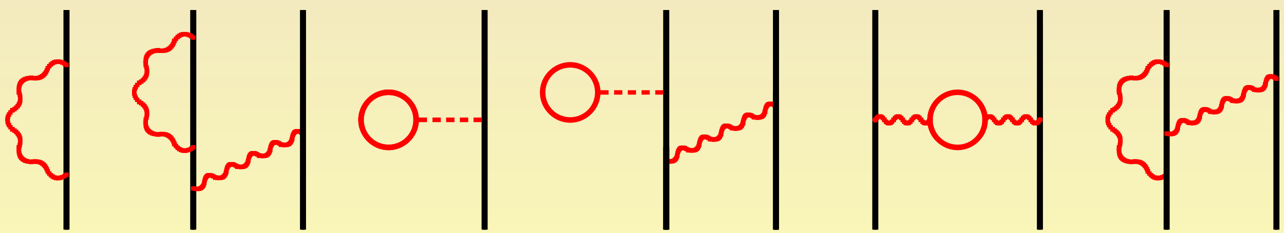
Effects beyond NVPA referred to as QED effects

- **Non-radiative effects (retardation, virtual pairs)**



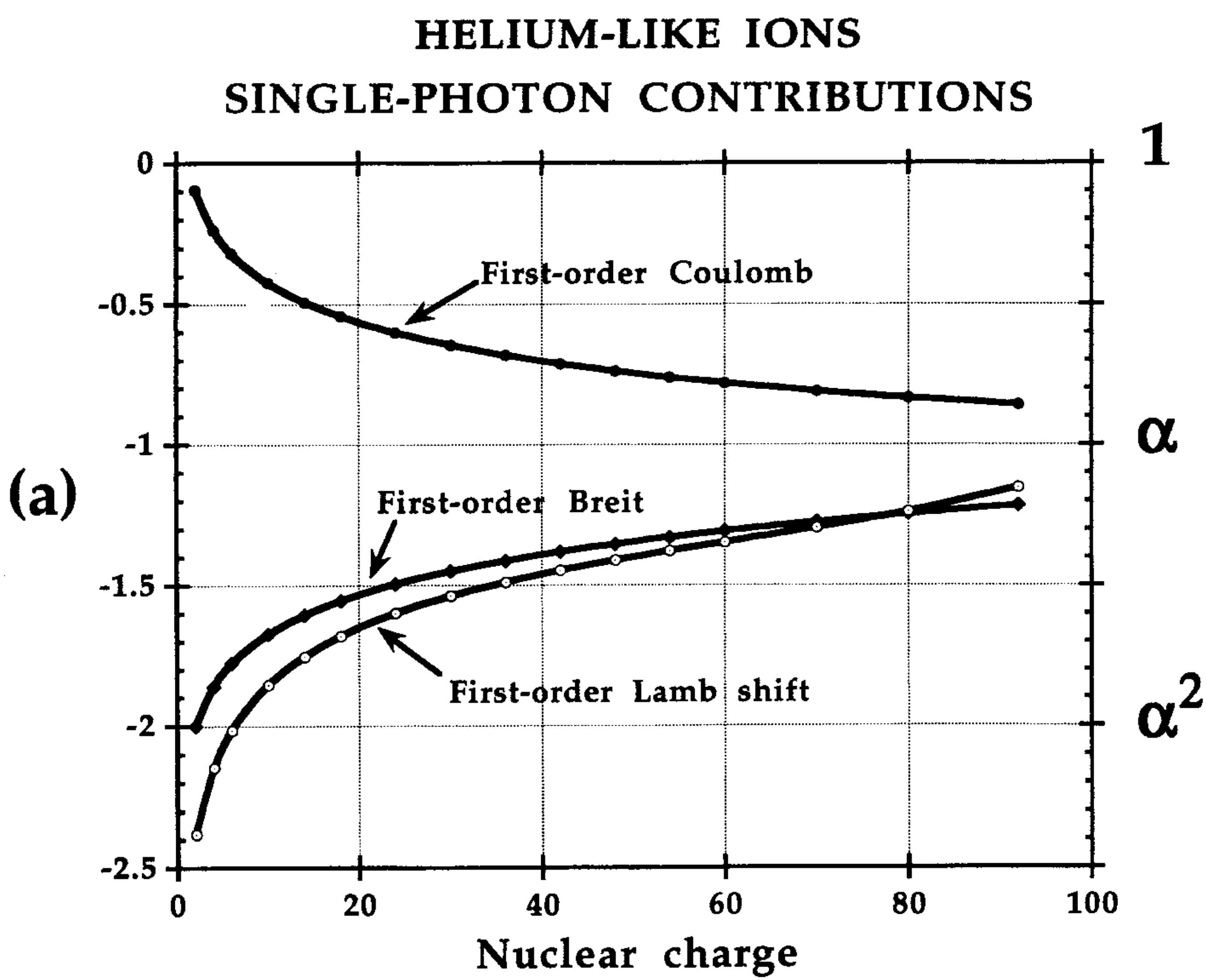
Retarded Breit   Araki-Sucher

- **Radiative effects**

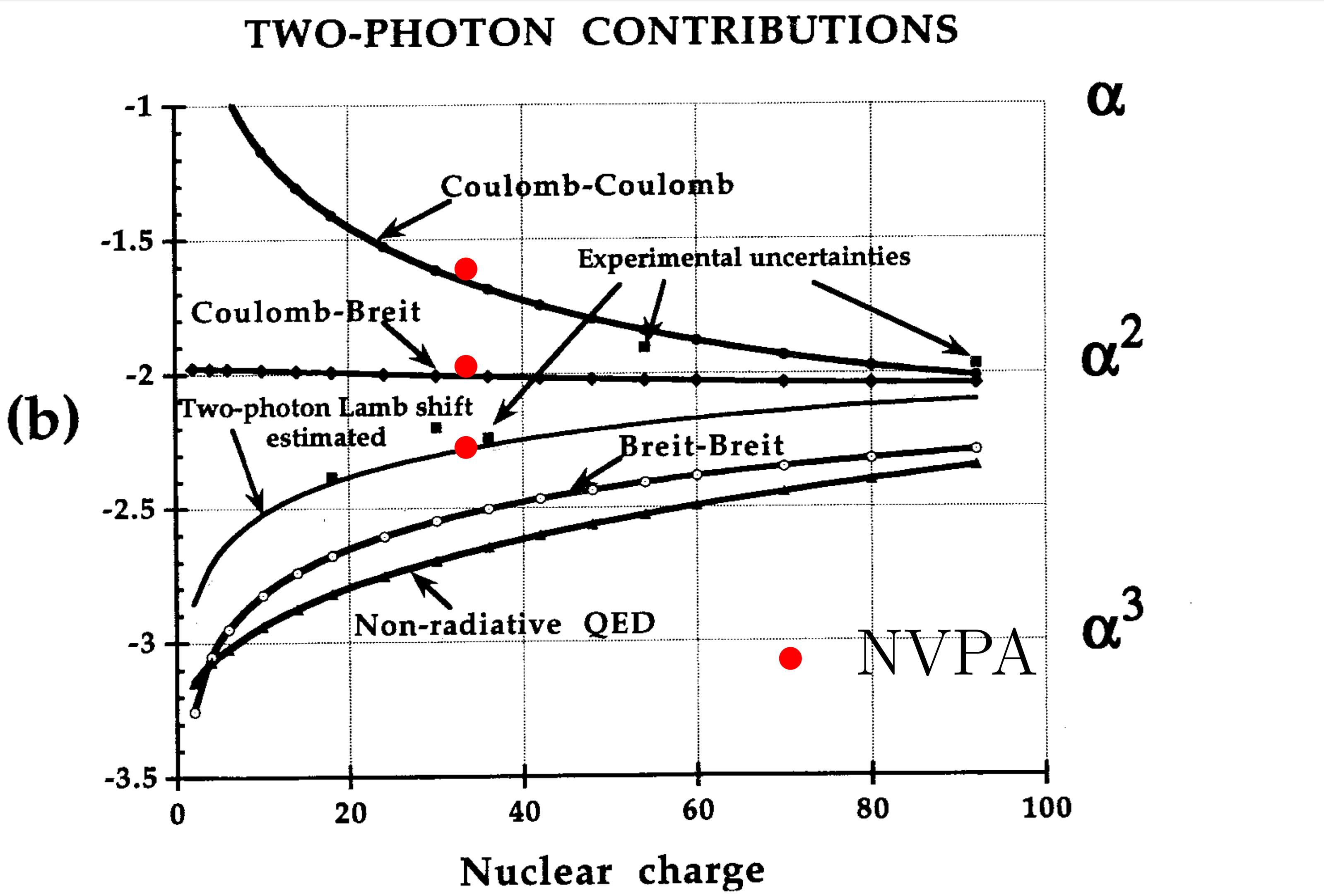


Self energy   Vacuum polarization   Vertex corr.

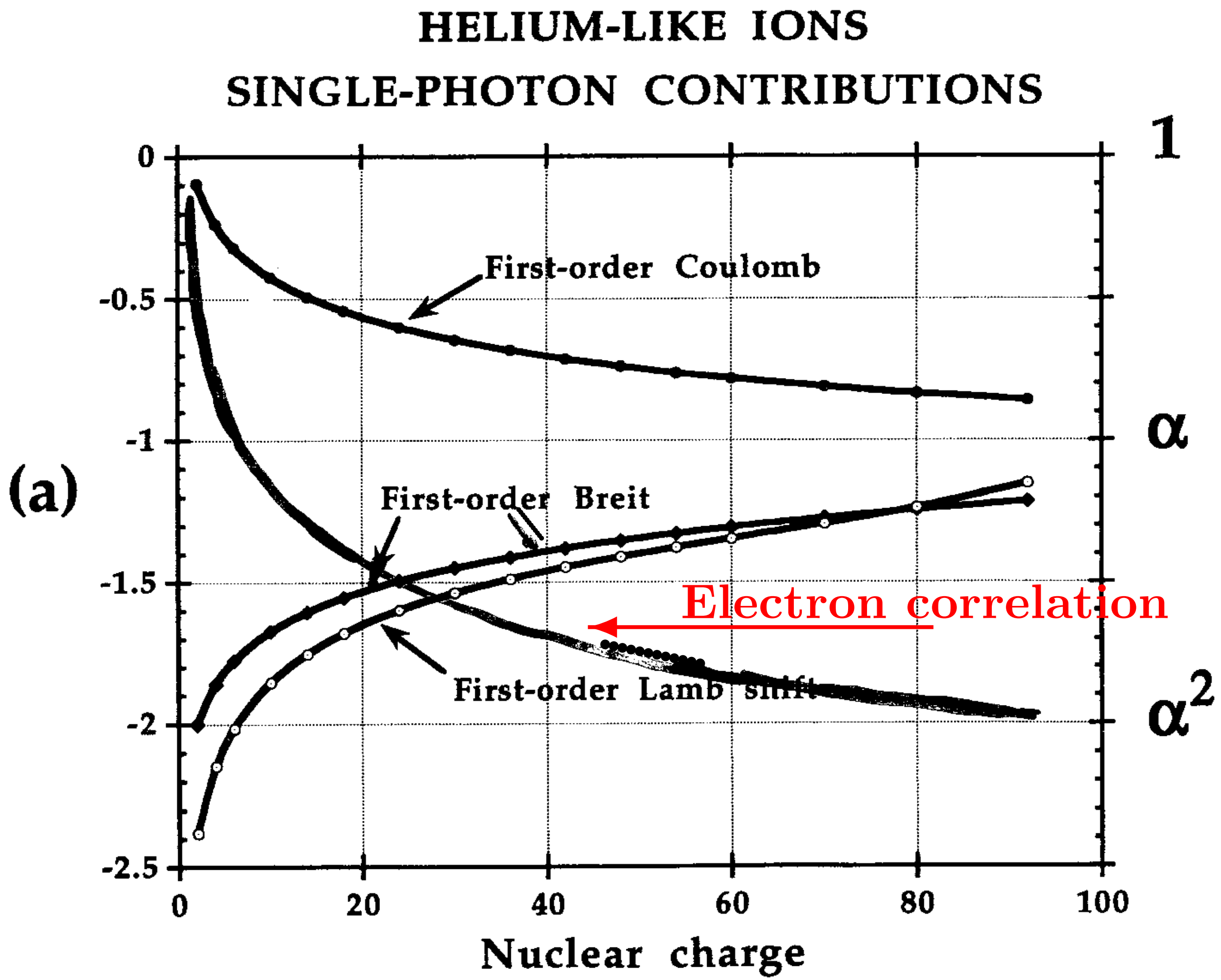
Need for a Many-Body-QED Procedure



Need for a Many-Body-QED Procedure



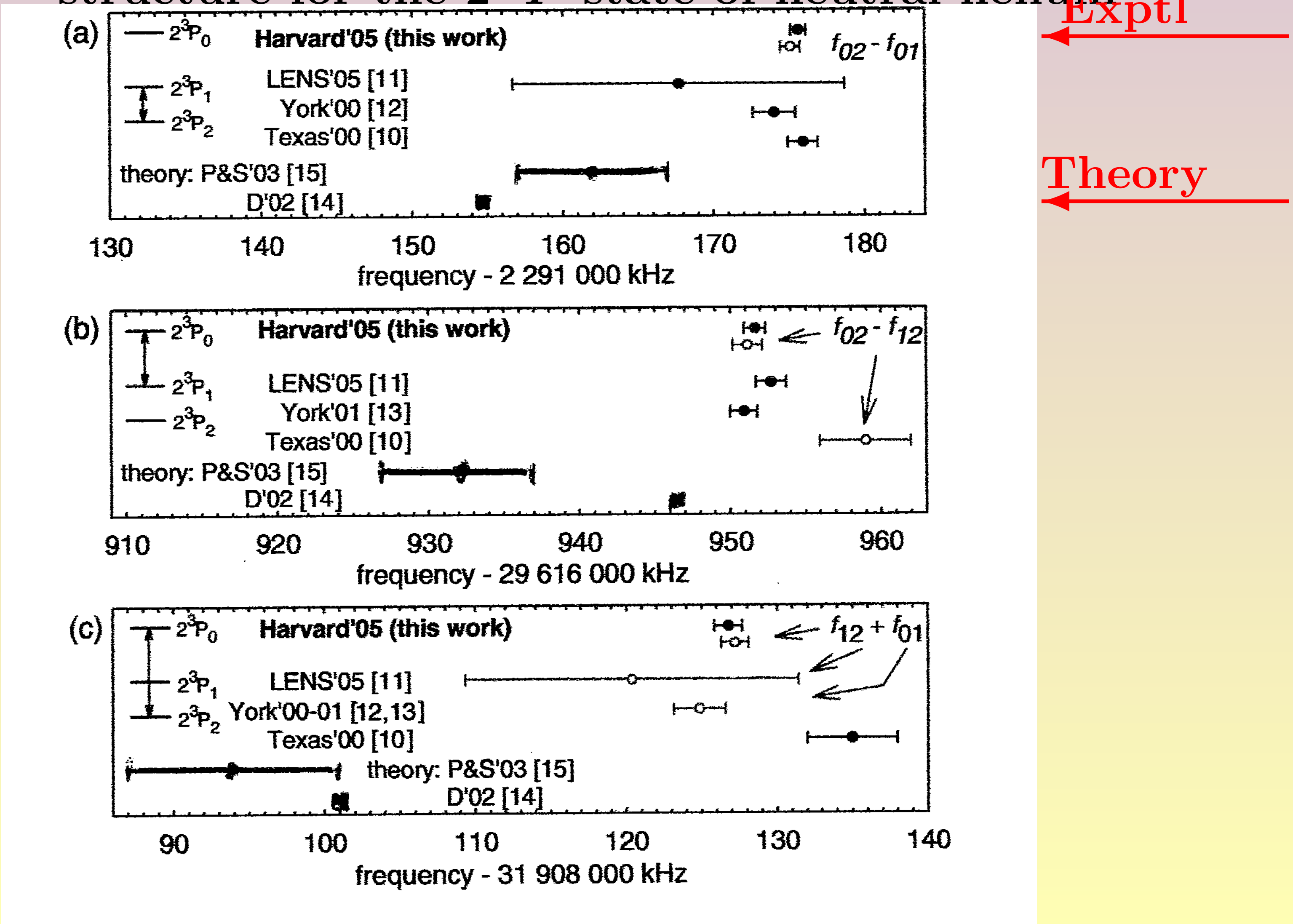
Need for a Many-Body-QED Procedure



Need for a Many-Body-QED Procedure

- **Most challenging are QED calculations on the lightest systems, where combined QED-correlation effects are most important**
- **A crucial test is the fine structure of neutral helium, which has been measured to a few ppb** (Gabrielse et al. PRL **95**, 20301, 2005)

Comparison between experimental and theoretical fine structure for the $2\,^3P$ state of neutral helium



Analytical calculations have failed to reproduce the helium fine structure

Can a "unified" numerical method improve the situation?

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Time-independent Many-Body Perturbation Theory

(Lindgren-Morrison: Atomic Many-Body Theory, Springer 1986)

Multi-reference case

Target states

$$H\,\Psi^{\alpha} = E^{\alpha}\,\Psi^{\alpha}\,; \qquad (\alpha = 1, 2, \cdots d)$$

$$H = H_0 + H'$$

Model states (intermediate normalization)

$$\Psi_0^{\alpha} = P\Psi^{\alpha}$$

Wave operator

$$\boxed{\Psi^{\alpha} = \Omega\,\Psi_0^{\alpha}}$$

The same for all reference states

Effective Hamiltonian

Project the Schrödinger eqn onto the model space:

$$P: \; H\,\Psi^{\alpha} = E^{\alpha}\,\Psi^{\alpha}$$

$$PH\Omega\Psi_0^{\alpha} = PE\Psi^{\alpha}$$

$$\boxed{H_{\text{eff}}\,\Psi_0^{\alpha} = E^{\alpha}\,\Psi_0^{\alpha}}$$

$$\boxed{H_{\text{eff}} = PH\Omega P = PH_0P + V_{\text{eff}}}$$

$V_{\text{eff}} = PH'\Omega P$ is the ***effective interaction***

$H_{\text{eff}}, V_{\text{eff}}$ generally multi-dimensional matrices

Time-independent MBPT

Generalized Bloch equation

(multi-reference) (Lindgren 1974)

$$\boxed{[\Omega, H_0]P = (H'\Omega - \Omega V_{\text{eff}})P}$$

Generates the generalized Rayleigh-Schrödinger pert. exp. The Brueckner-Goldstone linked-diagram expansion The Coupled-Cluster expansion

The wave operator and the effective Hamiltonian are the key ingredients of multi-reference many-body perfurbation theory.

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Time-dependent perturbation theory

Time-evolution operator

Interaction picture

$$\Psi_{\mathrm{I}}(t) = \mathrm{e}^{\mathrm{i}H_0 t}\Psi_{\mathrm{S}}(t)\,; \qquad O_{\mathrm{I}}(t) = \mathrm{e}^{\mathrm{i}H_0 t} O_{\mathrm{S}}\, \mathrm{e}^{-\mathrm{i}H_0 t}$$

$$\Psi_{\mathrm{I}\gamma}(t) = U_\gamma(t, t_0)\, \Psi_{\mathrm{I}\gamma}(t_0)$$

Adiabatic damping

$$H'_{\mathrm{I}}(t) \rightarrow H'_{\mathrm{I}\gamma}(t) = H'_{\mathrm{I}}(t)\,\mathrm{e}^{-\gamma|t|}$$

$$U_\gamma(t,t_0) = 1 + \sum_{n=1}^{\infty} \frac{(-\mathrm{i})^n}{n!} \int_{t_0}^{t} \mathrm{d}^4x_n \cdots \int_{t_0}^{t} \mathrm{d}^4x_1$$
$$\times T_{\mathrm{D}}\big[\mathcal{H}'_{\mathrm{I}}(x_n)\mathcal{H}'_{\mathrm{I}}(x_{n-1})\cdots\mathcal{H}'_{\mathrm{I}}(x_1)\big]\,\mathrm{e}^{-\gamma(|t_1|+\cdots+|t_n|)}$$

$$H'_{\mathrm{I}}(t) = \int \mathrm{d}^3x\,\mathcal{H}'_{\mathrm{I}}(t,x)$$

Evolution operator singular as $\gamma \rightarrow 0$

Gell-Mann–Low theorem (1951)

Single reference

$$\Psi = \lim_{\gamma\to 0} \Psi_{I\gamma}(t=0) = \lim_{\gamma\to 0} \frac{U_\gamma(0,-\infty)\Psi_0}{\langle\Psi_0|U_\gamma(0,-\infty)|\Psi_0\rangle}$$

Denominator eliminates singularities

(Linked-diagram theorem)

Satisfies the time-independent Schrödinger equation

(Single-reference case)

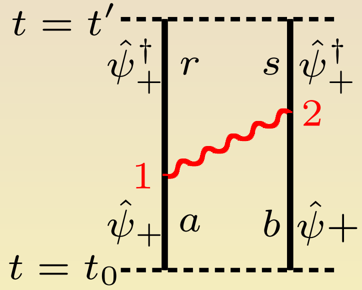
$$\boxed{\left(H_0 + H'\right)\Psi = E\,\Psi}$$

H' is time-independent in Schrödinger picture.

Single-photon exchange

Interaction between the electrons and the electro-magnetic radiation field: $\boldsymbol{\mathcal{H}'_{\mathrm{I}}(x) = -\hat{\psi}^{\dagger}_{\mathrm{I}}\alpha^{\mu}A_{\mu}\hat{\psi}_{\mathrm{I}}}$

TWO interactions represent the interaction between the electrons



$$U^{(2)}_{\gamma}(t', t_0) = -\frac{1}{2}\iint_{t_0}^{t'} \mathrm{d}^4x_1\mathrm{d}^4x_2\,\hat{\psi}^{\dagger}_{\mathrm{I}+}(x_1)\hat{\psi}^{\dagger}_{\mathrm{I}+}(x_2)$$

$$\times \mathrm{i}V_{sp}(x_1 - x_2)\,\hat{\psi}_{\mathrm{I}+}(x_2)\hat{\psi}_{\mathrm{I}+}(x_1)\,\mathrm{e}^{-\gamma(|t_1|+|t_2|)}$$

Time-dependent MBPT

$$V_{sp}(x_1 - x_2) = \alpha^\mu \alpha^\nu D_{F\mu\nu}(x_1 - x_2)$$

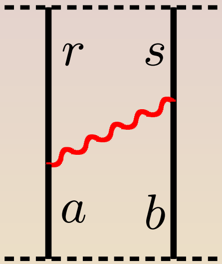
is the equivalent potential for single-photon exchange

$$D_{F\mu\nu}(x_1 - x_2) = -\mathrm{i} A_\mu(x_1) A_\nu(x_2)$$

is the Feynman photon propagator

S-matrix formulation

$$\boldsymbol{S = U(\infty, -\infty)}$$



In the limit $\gamma \to 0$

$$\langle rs \left| S^{(2)} \right| ab \rangle = -2\pi\mathrm{i}\,\delta(q + q')\,\langle rs | V_{sp}(q) | ab \rangle$$

$$q = \varepsilon_a - \varepsilon_r \;, q' = \varepsilon_b - \varepsilon_s$$

$$q + q' = \varepsilon_a + \varepsilon_b - \varepsilon_r - \varepsilon_s = 0$$

$V_{sp}(q)$ **is the Fourier transform of the single-photon potential**

Energy contribution given by

$$\Delta E = \delta_{q,-q'} \, \langle rs \big| V_{sp}(q) \big| ab \rangle$$

Energy conservation

In Coulomb gauge:

$$V_{sp}^{C}(q) = \frac{1}{r_{12}} + \int_0^{\infty} \frac{2k\,\mathrm{d}k\, f_C(k)}{q^2 - k^2 + \mathrm{i}\eta}$$

$$f_C(k) = \alpha_1 \cdot \alpha_2 \, \frac{\sin(kr_{12})}{\pi r_{12}} - (\alpha_1 \cdot \nabla_1)(\alpha_2 \cdot \nabla_2)\, \frac{\sin(kr_{12})}{\pi k^2 r_{12}}$$

Instantaneous Coulomb and retarded Breit interaction

S-matrix

The S-matrix formulation works well for first- and second-order QED contributions

Equivalent to lowest-order electron correlation

Works only in single-reference case

Can not treat quasidegeneracy

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Covariant evolution operator

(Lindgren et al. PRA 2001, Phys. Rep. Jan. 2004)

Generalized Gell-Mann-Low theorem

$$\Psi^{\alpha} = \lim_{\gamma\to 0} \frac{N^{\alpha}\, U_{\gamma}(0,-\infty)\, \Phi^{\alpha}}{\langle \Phi^{\alpha} | U_{\gamma}(0,-\infty) | \Phi^{\alpha} \rangle}$$

$$\Phi^{\alpha} = \lim_{\gamma\to 0} \lim_{\gamma\to -\infty} \Psi^{\alpha}(t)$$

parent state

Satisfies the S.E. in the multi-reference case:

$$\left(H_0 + H'\right) \Psi^{\alpha} = E^{\alpha}\, \Psi^{\alpha}$$

Covariant evolution operator

The singular evolution operator can be separated into a regular and a singular part:

$$U_\gamma(t,-\infty)P = P + \widetilde{U}_\gamma(t,-\infty)PU_\gamma(0,-\infty)P$$

$\widetilde{U}_\gamma(t,-\infty)$ **regular: Reduced evolution operator**

Factorization theorem (t=0):

$$U_\gamma(\,0\,,-\infty)P = \big[1 + Q\widetilde{U}(\,0\,,-\infty)\big]\,PU_\gamma(0,-\infty)P \qquad (Q = 1 - P)$$

Gell-Mann: $\Psi^\alpha = \lim_{\gamma\to 0} \dfrac{N^\alpha\, U_\gamma(0,-\infty)\,\Phi^\alpha}{\langle\Phi^\alpha|U_\gamma(0,-\infty)|\Phi^\alpha\rangle} = \Omega P\Psi^\alpha$

$$\boxed{\Psi^\alpha = \big[1 + Q\widetilde{U}(\,0\,,-\infty)\big]\,P\,\frac{N^\alpha\, U_\gamma(0,-\infty)\,\Phi^\alpha}{\langle\Phi^\alpha|U_\gamma(0,-\infty)|\Phi^\alpha\rangle}}$$

wave operator **model function**

Covariant evolution operator

Wave operator

$$\boxed{\Omega = 1 + Q\widetilde{U}(0,-\infty)}$$

s **Effective interaction**

$$\boxed{V_{\rm eff} = P\Big[\,\mathrm{i}\frac{\partial}{\partial t}\,\widetilde{U}(t,-\infty)\Big]_{t=0} P}$$

$$H_{\rm eff} = PH_0P + V_{\rm eff}$$

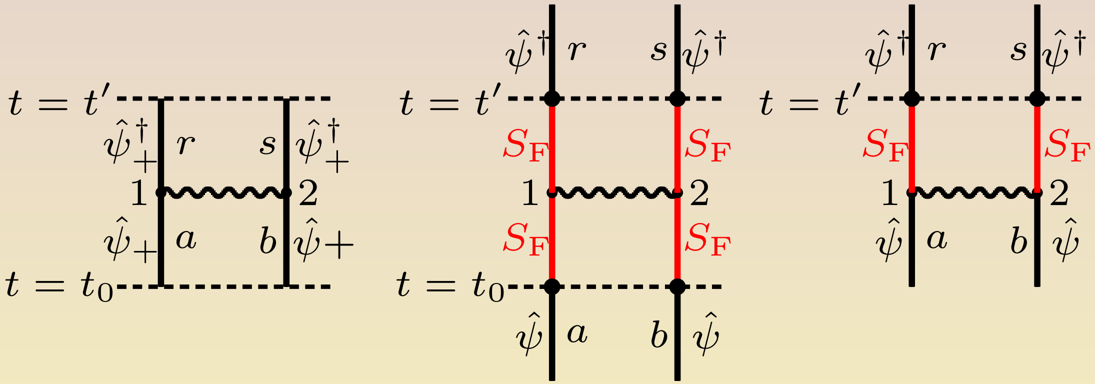
$\widetilde{U}(t,-\infty)$ **the regular part of the evolution operator**

Connection with standard MBPT

Covariant evolution operator

The standard evolution operator is non-covariant for finite times

It can be made covariant by inserting zeroth-order Green's functions



$$U^{(2)}_{\gamma\rm Cov}(t',t_0) = -\frac{1}{2} \quad d^3x'_1 d^3x'_2\, \hat\psi^\dagger_{\rm I}(x'_1)\hat\psi^\dagger_{\rm I}(x'_2)$$

$$d^4x_1 d^4x_2\, G_0(x'_1,x'_2;x_1,x_2) \quad d^3x_{10} d^3x_{20}\, {\rm i}V_{sp}(x_1,x_2)$$

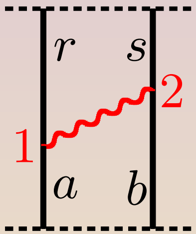
$$\times G_0(x_1,x_2;x_{10},x_{20})\, \hat\psi_{\rm I}(x_{20})\hat\psi_{\rm I}(x_{10})\, {\rm e}^{-\gamma(|t_1|+|t_2|)}$$

Integration of t_1 and t_2 over all times

Covariant evolution operator

Covariant-evolution operator for single-photon exchange

$$\left\langle rs \left| U^{(2)}_{\mathrm{Cov}}(t', -\infty) \right| ab \right\rangle = \frac{\mathrm{e}^{-\mathrm{i}t'(q+q')}}{q+q'} \left\langle rs \middle| V_{sp}(q, q') \middle| ab \right\rangle$$



$$q = \varepsilon_a - \varepsilon_r, \; q' = \varepsilon_a - \varepsilon_r$$

In Coulomb gauge:

$$V^C_{sp}(q, q') = \frac{1}{r_{12}} + \int_0^\infty f_C(k)\, \mathrm{d}k \left[\frac{1}{\mathrm{q} \mp (k - \mathrm{i}\eta)} + \frac{1}{\mathrm{q'} \mp (k - \mathrm{i}\eta)} \right]$$

$$f_C(k) = \boldsymbol{\alpha}_1 \cdot \boldsymbol{\alpha}_2 \, \frac{\sin(kr_{12})}{\pi r_{12}} - (\boldsymbol{\alpha}_1 \cdot \boldsymbol{\nabla}_1)(\boldsymbol{\alpha}_2 \cdot \boldsymbol{\nabla}_2) \, \frac{\sin(kr_{12})}{\pi k^2 r_{12}}$$

Note, potential has two parameters

Covariant evolution operator

The covariant-evolution-operator (Coul. gauge)

$$V_{sp}(\,\mathbf{q},\mathbf{q'}\,) = \frac{1}{r_{12}} + \int_0^\infty f(k)\,\mathrm{d}k \left[\frac{1}{\mathbf{q} \mp (k - \mathrm{i}\eta)} + \frac{1}{\mathbf{q'} \mp (k - \mathrm{i}\eta)} \right]$$

$$\langle rs\,|\Omega|\,ab\rangle = \frac{1}{q+q'}\,\langle rs|V_{sp}(q,q')|ab\rangle \quad (|rs\rangle \in Q)$$

$$\langle rs\,|V_{\mathrm{eff}}|\,ab\rangle = \langle rs|V_{sp}(q,q')|ab\rangle$$

Closely related to MBPT

C.f. S-matrix result:

$$V_{sp}(q) = \frac{1}{r_{12}} + \int_0^\infty \frac{2k\,\mathrm{d}k\,f(k)}{q^2 - k^2 + \mathrm{i}\eta}$$

$$\Delta E = \delta_{q,-q'}\,\langle rs|V_{sp}(q)|ab\rangle$$

No relation to wave operator

No off-diagonal elements of effective Hamiltonian

Fine-structure separations for He-like ions

lowest P state (in μ Hartree)

Including one- and two-photon exchange

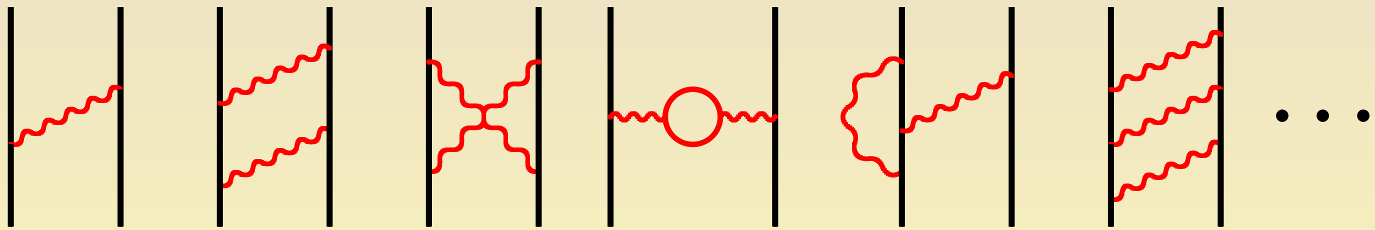
Ion	Transition	Expt'l	Åsén	Drake	Artemyev
Z=9	$^3P_2 -^3 P_1$	0,118761(1)	0,11875	0,11870	
Z=9	$^3P_1 -^3 P_0$	0,0191(2)	0,0188	0,0186	
Z=10	$^3P_2 -^3 P_0$	0,2302(1)	0,2302	0,2301	
Z=10	$^3P_1 -^3 P_0$	0,0373(2)	0,0373	0,0370	
Z=18	$^3P_2 -^3 P_0$	3,4003(8)	3,4003	3,3961	3.4000

The $^3P_1$ state is a quasi-degenerate combination of the states $1s2p_{1/2}$ and $1s2p_{3/2}$

How can we get further?

Including interactions to all orders is equiv. to exactly solving the Bethe-Salpeter eqn

$$\boxed{(E - H_0)\,\Psi = \mathcal{V}(E)}$$



Not feasible beyond two phot. with std methods

Poor treatment of electron correlation

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Including correlation

Gell-Mann–Low theorem (1951)

Single reference

$$\Psi = \lim_{\gamma\to 0} \Psi_{I\gamma}(t=0) = \lim_{\gamma\to 0} \frac{U_\gamma(0,-\infty)\Psi_0}{\langle\Psi_0|U_\gamma(0,-\infty)|\Psi_0\rangle}$$

Denominator eliminates singularities

(Linked-diagram theorem)

Satisfies the time-independent Schrödinger equation

(Single-reference case)

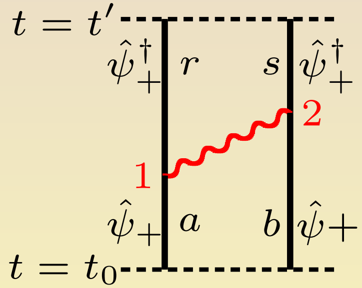
$$\boxed{\left(H_0 + H'\right)\Psi = E\,\Psi}$$

H' **is time-independent in Schrödinger picture.**

Single-photon exchange

Interaction between the electrons and the electro-magnetic radiation field: $\boldsymbol{\mathcal{H}'_{\mathrm{I}}(x) = -\hat{\psi}^{\dagger}_{\mathrm{I}}\alpha^{\mu}A_{\mu}\hat{\psi}_{\mathrm{I}}}$

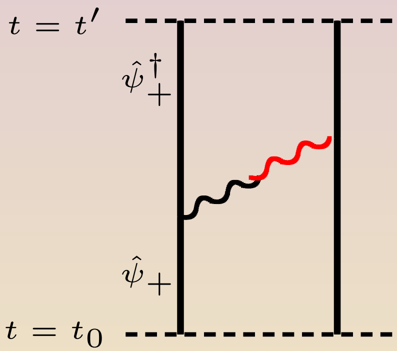
TWO interactions represent the interaction between the electrons



$$U^{(2)}_{\gamma}(t',t_0) = -\frac{1}{2}\iint_{t_0}^{t'} \mathrm{d}^4x_1\mathrm{d}^4x_2\,\hat{\psi}^{\dagger}_{\mathrm{I}+}(x_1)\hat{\psi}^{\dagger}_{\mathrm{I}+}(x_2)$$

$$\times\mathrm{i}V_{sp}(x_1-x_2)\,\hat{\psi}_{\mathrm{I}+}(x_2)\hat{\psi}_{\mathrm{I}+}(x_1)\,\mathrm{e}^{-\gamma(|t_1|+|t_2|)}$$

Extended Fock space



The intermediate states lie in Fock space

with variable number of photons

Satisfies the Fock-space-Schrödinger eqn

$$\big(H_0 + H'\big)\,\Psi = E\,\Psi \qquad \mathcal{H}'_{\mathrm{I}}(x) = -\hat{\psi}_{\mathrm{I}}^\dagger \alpha^\mu A_\mu \hat{\psi}_{\mathrm{I}}$$

Projection on Hilbert space gives (std, single-ref.)

Bethe-Salpeter eqn

$$\boxed{\big(E - H_0\big)\,\Psi = \mathcal{V}(E)}$$

Including correlation

The Bethe-Salpeter eqn

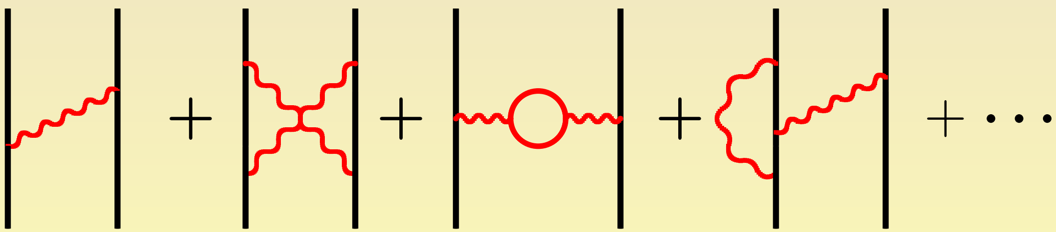
$$\boxed{\left(E - H_0\right)\Psi = \mathcal{V}(E)}$$

leads directly to the Brillouin-Wigner expansion

$$\Psi = \left[1 + \frac{1}{E-H_0}\mathcal{V}(E) + \frac{1}{E-H_0}\mathcal{V}(E)\frac{1}{E-H_0}\mathcal{V}(E) + \cdots\right]$$

The potential is given by all irreducible diagrams

$$\mathcal{V}(E) =$$



Including correlation

Bloch eqn valid in the extended Fock space

$$\boxed{[\Omega, H_0]P = \big(H'\Omega - \Omega\, V_{\text{eff}}\big)P}$$

Projection of this eqn on Hilbert space
gives the (multiref.) Bethe-Salpeter-Bloch eqn

$$\boxed{[\Omega, H_0]P = \mathcal{V}(H_{\text{eff}})\Omega - \Omega\, V_{\text{eff}}}$$

Einstein Centennial paper:
Lindgren, Salomonson, Hedendahl, Can.J.Phys. 83, 183 (2005)

Our equations have much simpler structure in Fock space

Including correlation

Fock space

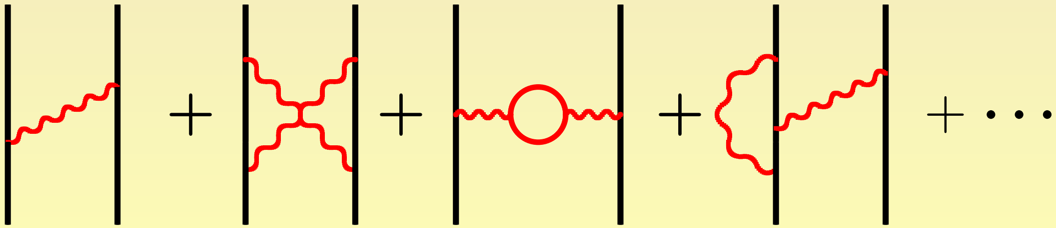
$$\boxed{\left(H_0 + H'\right)\Psi = E\,\Psi}$$

Perturbation is given by the energy-independent electron-field interaction density $\mathcal{H}'_{\mathrm{I}}(x) = -\hat{\psi}^{\dagger}_{\mathrm{I}}\alpha^{\mu}A_{\mu}\hat{\psi}_{\mathrm{I}}$

Hilbert space

$$\boxed{\left(E - H_0\right)\Psi = \mathcal{V}(E)}$$

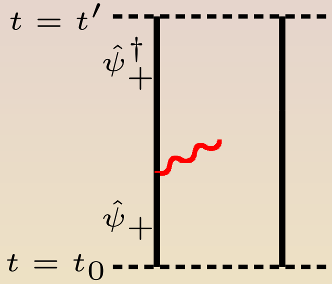
Perturbation is the energy-dependent potential

$\mathcal{V}(E) =$ 

Including correlation

Covariant-Evolution-Operator Approach

Including electron correlation



Treat single interaction as perturbation

with wave function in Fock space

$$\left(H_0 + H'\right)\Psi = E\,\Psi$$

Use the Bloch eqn in Fock space

$$\boxed{\left[\Omega, H_0\right]P = \left(H'\Omega - \Omega\, V_{\mathrm{eff}}\right)P}$$

Including correlation

Single-photon potential in Coulomb gauge

$$V_{sp}(q,q') = \frac{1}{r_{12}} + \int_0^\infty f_C(k)\,\mathrm{d}k \left[\frac{1}{q \mp (k - \mathrm{i}\eta)} + \frac{1}{q' \mp (k - \mathrm{i}\eta)} \right]$$

V_C $\quad\quad$ V_{sp}^{ret}

$$f_C(k) = \alpha_1 \cdot \alpha_2 \frac{\sin(kr_{12})}{\pi r_{12}} - (\alpha_1 \cdot \nabla_1)(\alpha_2 \cdot \nabla_2) \frac{\sin(kr_{12})}{\pi k^2 r_{12}}$$

Gaunt interaction $\quad\quad$ **scalar-retardation part**

$$\frac{\sin(kr_{12})}{kr_{12}} = \sum_{l=0}^{\infty} (2l+1) j_l(kr_1) j_l(kr_2) C^l(1) \cdot C^l(2)$$

$$\boxed{f_C(k) = \sum_{l=0}^{\infty} \left[V_G^l(kr_1) \cdot V_G^l(kr_2) - V_{\mathrm{SR}}^l(kr_1) \cdot V_{\mathrm{SR}}^l(kr_2) \right]}$$

Including correlation

Bloch equation

$$[\Omega, H_0]P = (H'\Omega - \Omega V_{\text{eff}})P$$

Perturbation

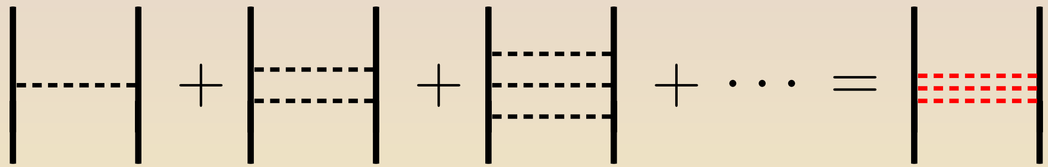
$$H' = V_C + V_+^l + V_-^l$$

Note, all terms are energy independent. The energy dependence originates from the commutator/energy denominator

This is the only perturbation needed

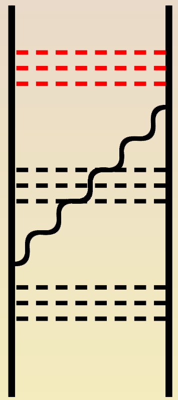
Including correlation

$$[\boldsymbol{\Omega}, \boldsymbol{H_0}]\boldsymbol{P} = \left(\boldsymbol{V_C} + \boldsymbol{V^l_+} + \boldsymbol{V^l_-}\right)\boldsymbol{\Omega P} - \boldsymbol{Folded}$$

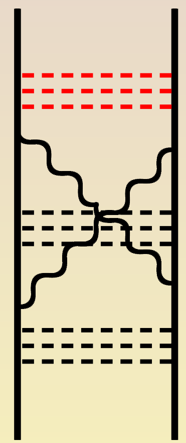


Including correlation

$$\left[\boldsymbol{\Omega}, \boldsymbol{H_0}\right]\boldsymbol{P} = \left(\boldsymbol{V_C} + \boldsymbol{V^l_+} + \boldsymbol{V^l_-}\right)\boldsymbol{\Omega P} - \boldsymbol{Folded}$$



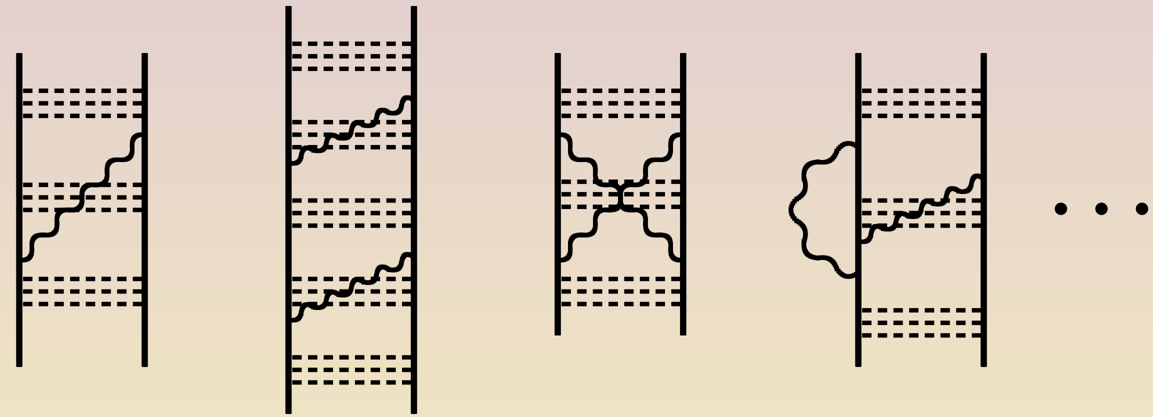
The procedure can also be used for multi-photon effects



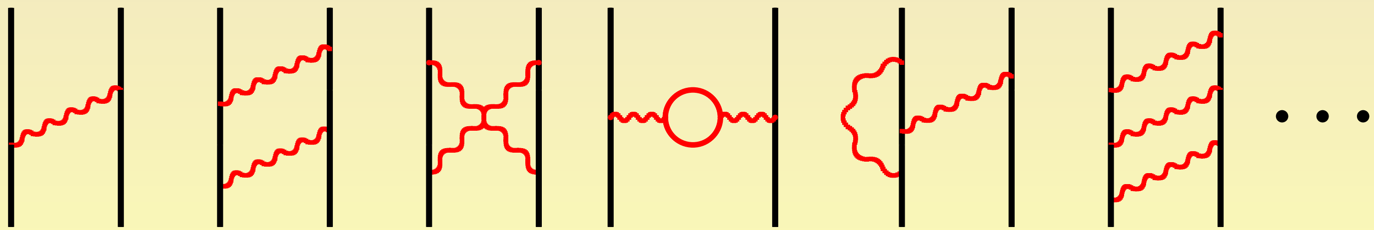
although this is computationally very demanding

Including correlation

Expanding the one-, two-,...photon interactions with correlation leads to a much faster convergence towards the Bethe-Salpeter eqn



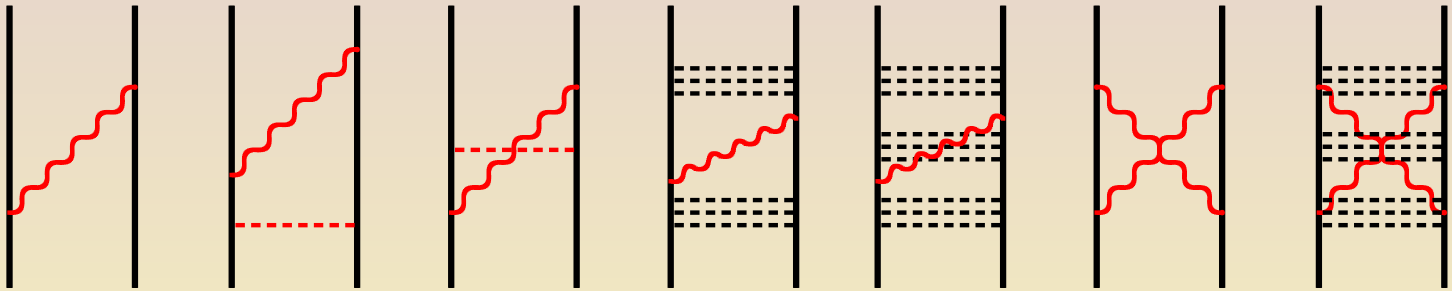
Compare



Numerical results

Heliumlike neon, 1s2s ^1S

Energy contributions beyond relativistic MBPT



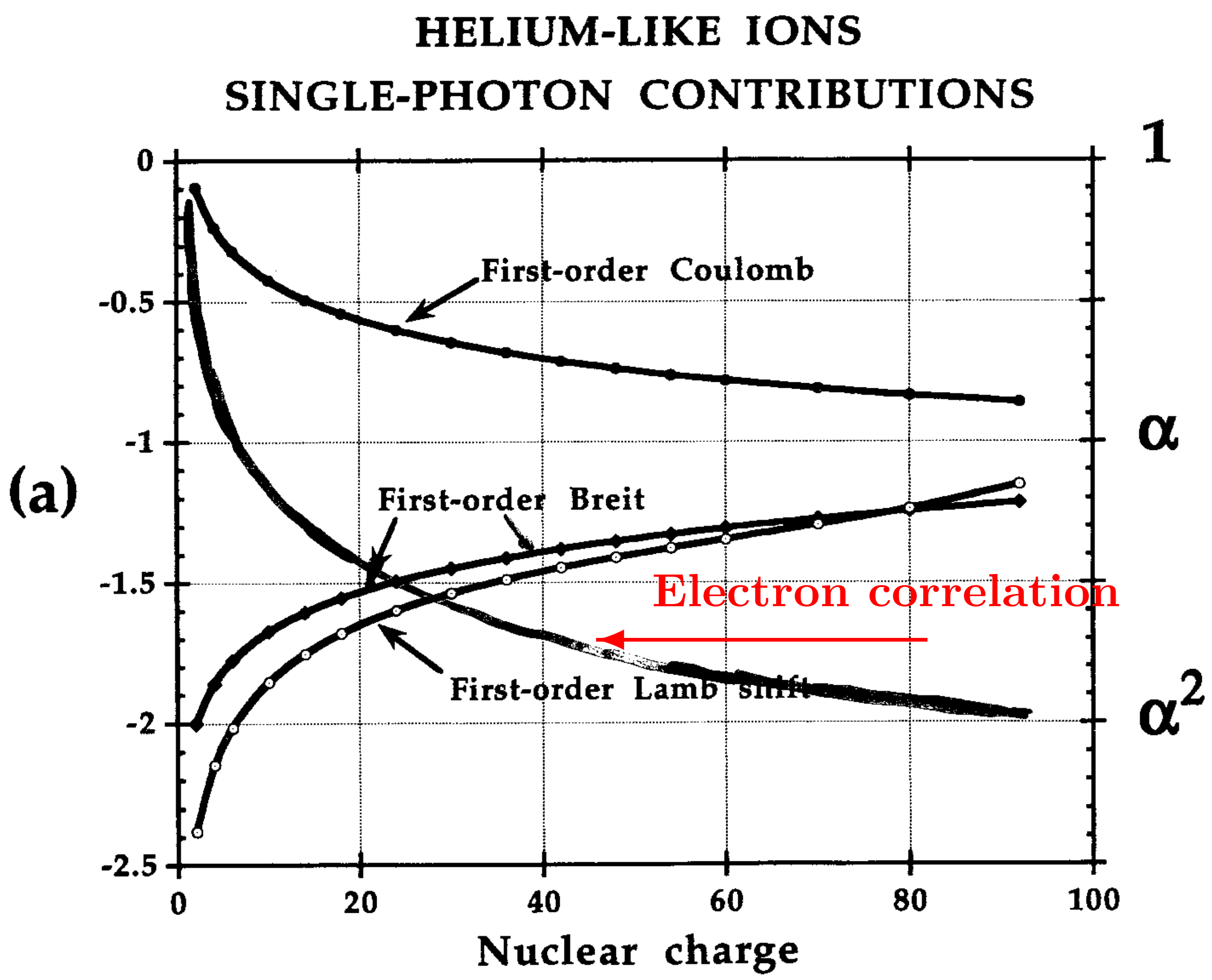
2637 μH -773 -18 **72** **$\sim$-5** -7 1-2 μH

The correlation part represents 25% of the effect

Summary and Conclusions

- **For heavy, highly charged ions relativistic and QED effects dominate over electron correlation**
- **For light systems electron correlation dominates and combined QED-correlation effects might be significant**

Summary and Conclusions



Summary and Conclusions

- **For heavy, highly charged ions relativistic and QED effects dominate over electron correlation**
- **For light systems electron correlation dominates and combined QED-correlation effects might be significant**
- **S-matrix standard method for QED calculations— works well for highly charged ions but not for lighter systems**
  Cannot treat multi-reference case (quasi-degeneracy)
- **Covariant-evolution-operator method QED technique developed for multi-reference case**

Summary and Conclusions

The covariant-evolution-operator (Coul. gauge)

$$V_{sp}(q,q') = \frac{1}{r_{12}} + \int_0^\infty f(k)\,\mathrm{d}k \left[\frac{1}{q\mp(k-\mathrm{i}\eta)} + \frac{1}{q'\mp(k-\mathrm{i}\eta)}\right]$$

$$\langle rs\,|\Omega|\,ab\rangle = \frac{1}{q+q'}\,\langle rs\big|V_{sp}(q,q')\big|ab\rangle \quad (|rs\rangle \in Q)$$

$$\langle rs\,|V_{\text{eff}}|\,ab\rangle = \langle rs\big|V_{sp}(q,q')\big|ab\rangle$$

Closely related to MBPT

C.f. S-matrix result:

$$V_{sp}(q) = \frac{1}{r_{12}} + \int_0^\infty \frac{2k\,\mathrm{d}k\,f(k)}{q^2-k^2+\mathrm{i}\eta}$$

$$\Delta E = \delta_{q,-q'}\,\langle rs\big|V_{sp}(q)\big|ab\rangle$$

No relation to wave operator

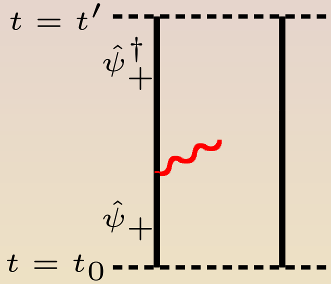
No off-diagonal elements of effective Hamiltonian

Summary and Conclusions

- **For heavy, highly charged ions relativistic and QED effects dominate over electron correlation**
- **For light systems electron correlation dominates and combined QED-correlation effects might be significant**
- **S-matrix standard method for QED calculations— works well for highly charged ions but not for lighter systems Cannot treat multi-reference case (quasi-degeneracy)**
- **Covariant-evolution-operator method QED technique developed for multi-reference case**
- **By treating field interaction with single electron as perturbation in Fock space, electron correlation could be included. Leads to faster convergence towards the Bethe-Salpeter eqn.**

Covariant-Evolution-Operator Approach

Including electron correlation



Treat single interaction as perturbation

with wave function in Fock space

$$\left(H_0 + H'\right)\Psi = E\,\Psi$$

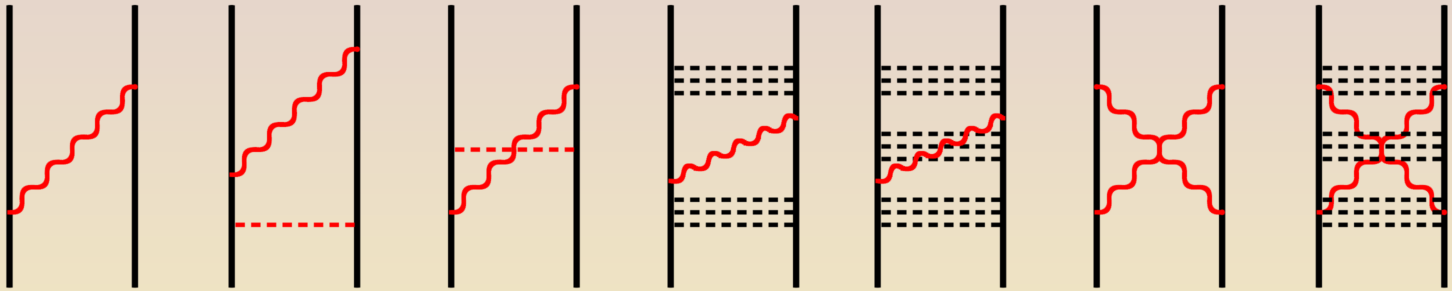
Use the Bloch eqn in Fock space

$$\boxed{\left[\Omega, H_0\right]P = \left(H'\Omega - \Omega\, V_{\text{eff}}\right)P}$$

Numerical results

Heliumlike neon, 1s2s ^1S

Energy contributions beyond relativistic MBPT



2637 μH	-773	-18	**72**	**$\sim$-5**	-7	1-2 μH

The correlation part represents 25% of the effect

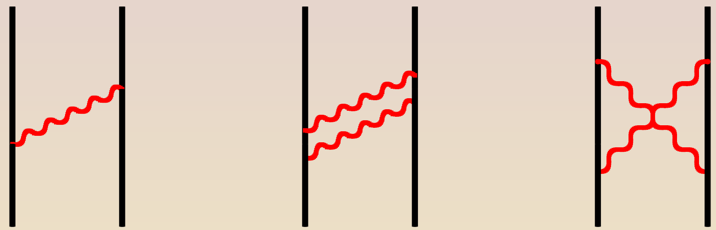
Outlook

- The new technique can lead to more accurate QED calculations
  on light and medium-heavy systems
- The technique is for computational reasons at present limited to few-electron systems
- So far, only non-radiative effects have been evaluated. Evaluation of radiative effects is in preparation
- A good testing case is the fine structure of He-like ions

Outlook

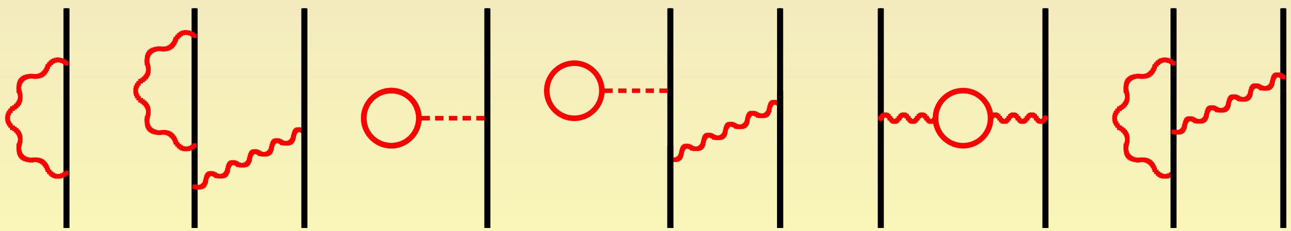
Effects beyond NVPA referred to as QED effects

- **Non-radiative effects** (retardation, virtual pairs)



Retarded Breit   Araki-Sucher

- **Radiative effects** (self energy, vacuum polarization, vertex corrections)



Self energy   Vacuum polarization   Vertex corr.

Outlook

- **The new technique can lead to more accurate QED calculations on light and medium-heavy systems**
- **The technique is for computational reasons at present limited to few-electron systems**
- **So far, only non-radiative effects have been evaluated. Evaluation of radiative effects is in preparation**
- **A good testing case is the fine structure of He-like ions**

Fine-structure separations for He-like ions

Lowest P state (in μ Hartree)

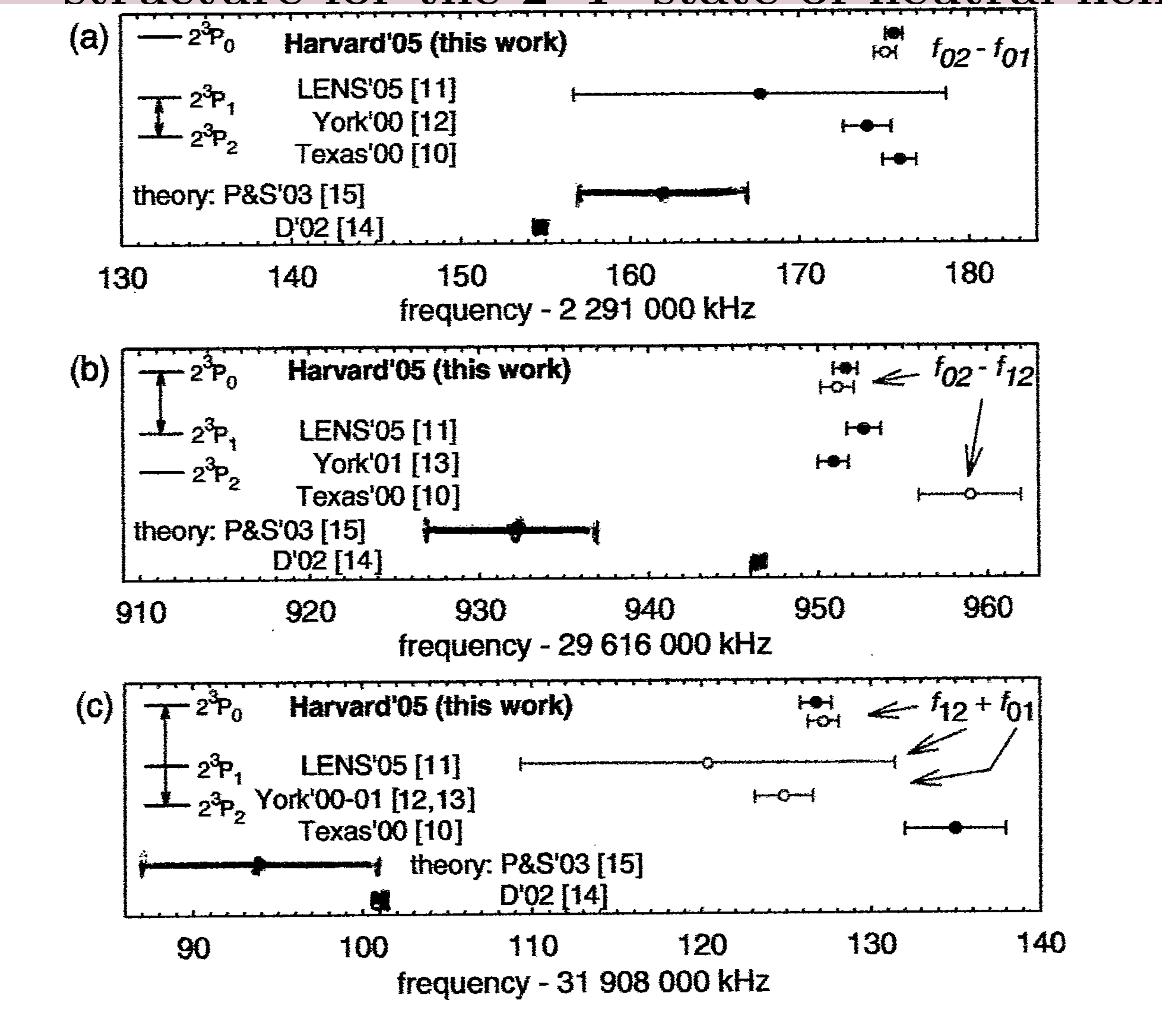
Ion	Transition	Expt'l	Åsén	Drake	Artemyev
Z=9	$^3P_2 -^3 P_1$	**0,118761(1)**	0,11875	0,11870	
Z=9	$^3P_1 -^3 P_0$	0,0191(2)	0,0188	0,0186	
Z=10	$^3P_2 -^3 P_0$	0,2302(1)	0,2302	0,2301	
Z=10	$^3P_1 -^3 P_0$	0,0373(2)	0,0373	0,0370	
Z=18	$^3P_2 -^3 P_0$	3,4003(8)	3,4003	3,3961	3.4000

The $^3P_1$ state is a quasi-degenerate combination of the states $1s2p_{1/2}$ and $1s2p_{3/2}$

Outlook

- **Most challenging are QED calculations on the lightest systems, where combined QED-correlation effects are most important**
- **A crucial test is the fine structure of neutral helium, which has been measured to a few ppb** (Gabrielse et al. PRL **95**, 20301, 2005)

Comparison between experimental and theoretical fine structure for the $2\,^3P$ state of neutral helium



Exptl

Theory

Outlook

Analytical calculations have failed to reproduce the helium fine structure

We believe that a "unified" numerical method can be constructed for heavy as well as light systems!

Coworkers

Sten Salomonson
Björn Åsén
Daniel Hedendahl

Recent publications

- **I.Lindgren, S.Salomonson, and B.Åsén, Physics Reports, 389, 161 (2004)**
- **I.Lindgren, S.Salomonson and D.Hedendahl, Can. J. Phys. 83, 183 (2005)** ("Einstein Centennial paper")
- **I.Lindgren, S.Salomonson and D.Hedendahl, Phys. Rev. A73, 062502 (2006)**