MBTP for energy-dependent interactions

A road towards a merger of MBPT and QED

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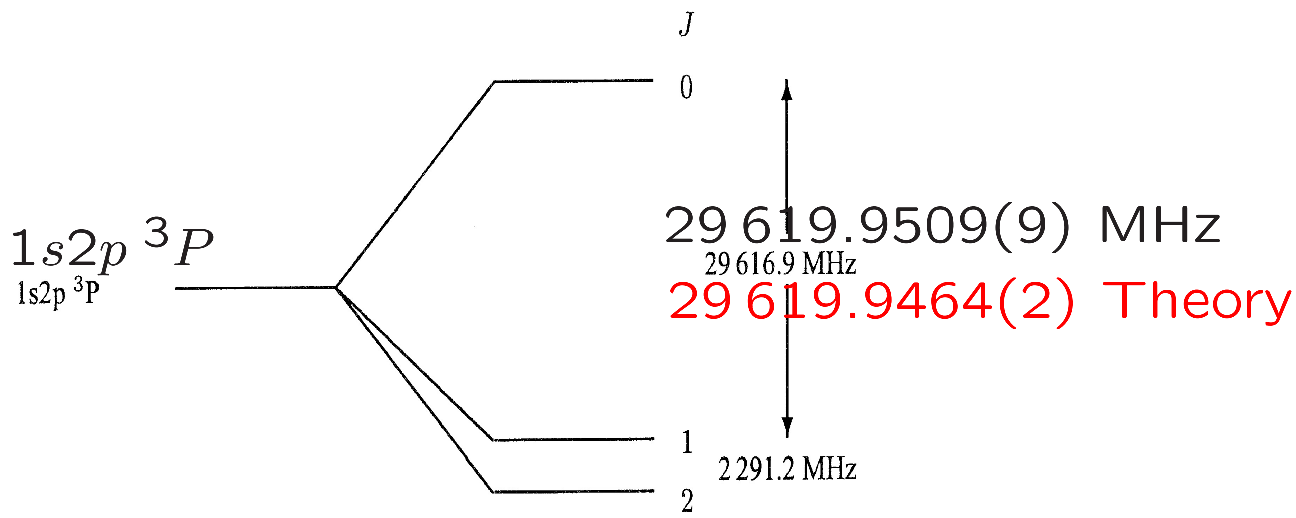
Outline

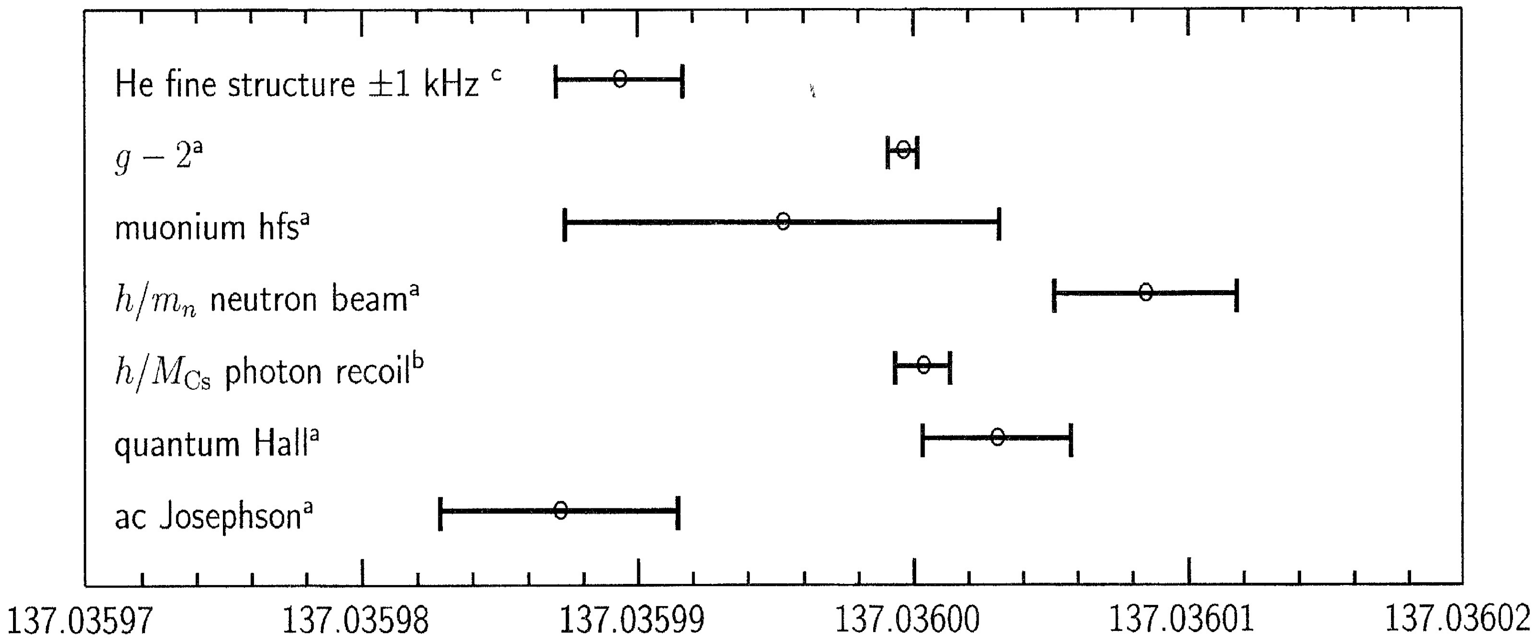
- Introduction (Helium fine structure)
- Bethe-Salpeter approach
- S-matrix and the evolution operator method
- Energy-dependent MBPT – MBPT-QED merger
- Numerical approach

Fine structure of helium atom (2002)



Fine-structure constant

(from Drake, Can. J. Phys. **80**, 1195 (2002))



CODATA 2002

Inguscio 2004

Paris 2005

Deviation theory-exp: 7 std dev

Helium fine structure:
A challenging theoretical problem

Involves:

MBPT/CCA

S-matrix

Strong correlation

High-order QED

Quasi-degeneracy

Cov.Ev.Op.

The Bethe-Salpeter approach

Dyson equation for the Green's function

$$G = G_0 + G_0 \kappa G$$

$$\mathrm{i} G_0(E) = \frac{1}{E - H_0} \left(\Lambda_{++} - \Lambda_{--} \right)$$

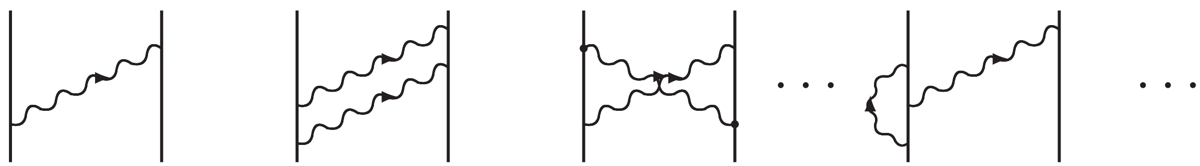
Using plane waves, the homogeneous part represents the

bound-state wave function

$$\boxed{\Psi = G_0 \kappa \Psi}$$

Bethe-Salpeter equation

κ **represents all irreducible kernels**



BS equation can be expressed in the form

$$(\boldsymbol{E} - \boldsymbol{H_c})\boldsymbol{\Psi}(\boldsymbol{E}) = \boldsymbol{\mathcal{V}}_{\mathbf{QED}}\boldsymbol{\Psi}(\boldsymbol{E})$$

$$H_c = H_0 + \Lambda_{++} I_c \Lambda_{++}$$

Sucher "no-pair" Hamiltonian

Treated by means of Brillouin-Wigner perturbation expansion

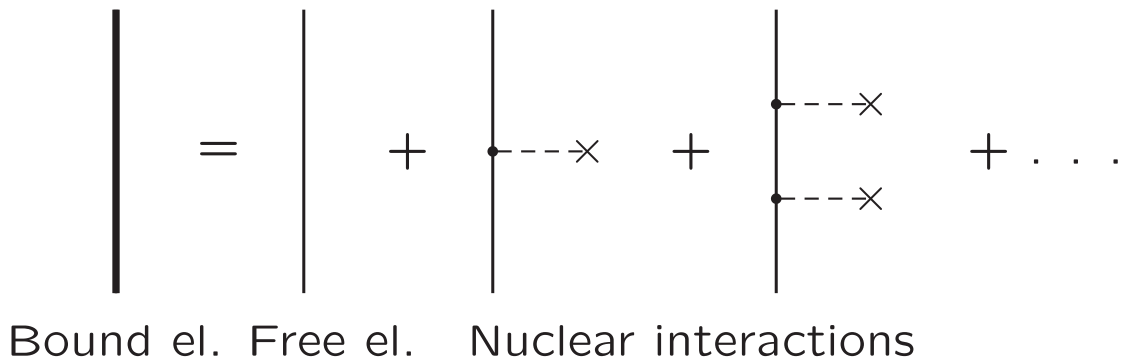
$$\boldsymbol{E} = \boldsymbol{E_c} + \langle \boldsymbol{\Psi_c} | \boldsymbol{\mathcal{V}}_{\mathbf{QED}} + \boldsymbol{\mathcal{V}}_{\mathbf{QED}} \boldsymbol{\Gamma_Q} \boldsymbol{\mathcal{V}}_{\mathbf{QED}} + \boldsymbol{\mathcal{V}}_{\mathbf{QED}} \boldsymbol{\Gamma_Q} \boldsymbol{\mathcal{V}}_{\mathbf{QED}} \boldsymbol{\Gamma_Q} \boldsymbol{\mathcal{V}}_{\mathbf{QED}} + \cdots | \boldsymbol{\Psi_c} \rangle$$

$$\Gamma_Q = \frac{Q}{E - H_c}$$

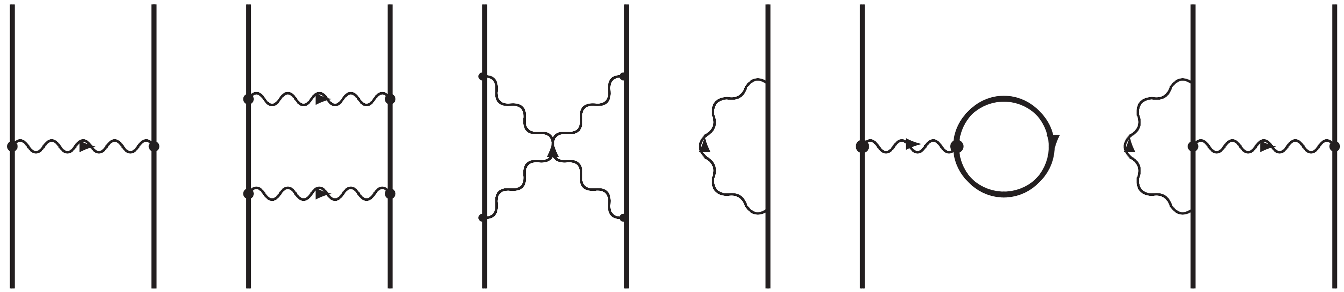
Sucher 1957, Douglas-Kroll 1974, Zhang-Drake 1996

S-matrix approach to energy-dependent interactions

1. **Start from hydrogenic Dirac orbitals (Green's functions) in nuclear potential (Furry picture)**



2. Evaluate one-, two-, ... photon exchange energies



Non-radiative Radiative

Applied mainly to heavy elements
Only one- and two-photon exchange can be evaluated
Electron correlation poorly treated

Energy conservation
Not applicable to quasi-degeneracy

No information about wave function
No connection to MBPT

Standard MBPT

1. **Model space** (P)

Strongly mixed states included in the model space
Important for **quasi-degeneracy** (fine structure).

2. **Wave operator** (Ω)

$$\Psi^\alpha = \Omega\, \Psi_0^\alpha \qquad \Psi_0^\alpha = P\Psi^\alpha \qquad (\alpha = 1, 2, \cdots d)$$

3. **Effective Hamiltonian** (H_{eff})

$$H_{\text{eff}} = PH_0P + H'_{\text{eff}} \qquad H'_{\text{eff}} = PV\Omega P$$

$$H_{\text{eff}}|\Psi_0^\alpha\rangle = E^\alpha|\Psi_0^\alpha\rangle$$

Wave operator satisfies the Bloch eqn

$$\big(E_0 - H_0\big)\Omega P = V\,\Omega P - \Omega\,H'_{\text{eff}} \qquad (V = 1/r_{12})$$

$$\big[\Omega, H_0\big]P = V\,\Omega P - \Omega\,H'_{\text{eff}}$$

Linked-diagram theorem:

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

The Bloch eqn in commutator form can handle

quasi-degeneracy

The Bloch eqn can also be used to generate

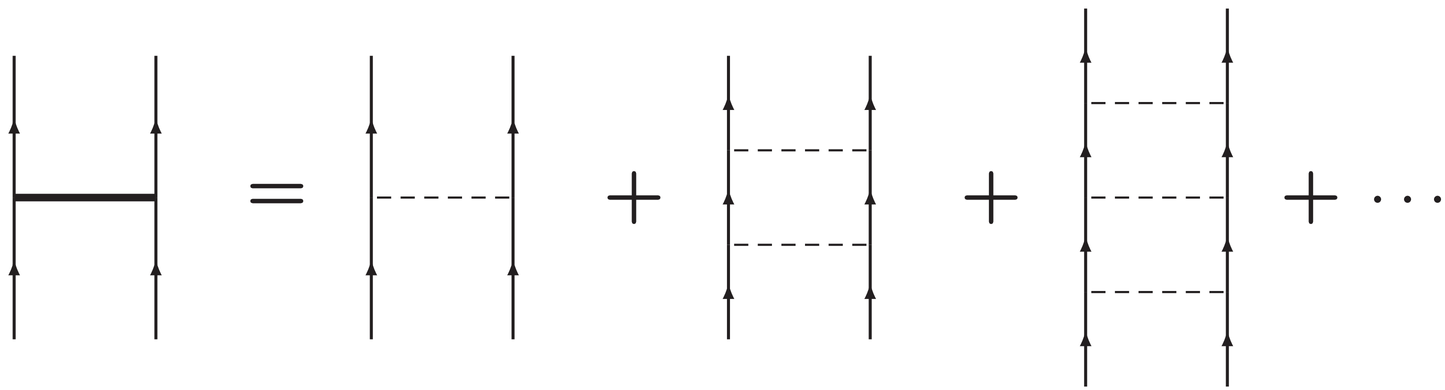
all-order MBPT procedures

Coupled-Cluster Approach

$$\Omega = \{e^{S}\} \qquad S = S_1 + S_2 + \cdots$$

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

Pair function (S_2)



Includes pair correlation to all orders

MBPT/CCA can handle quasi-degeneray and correlation effects to all orders for energy-independent interactions.

What about energy-dependent interactions, like QED?

Time-dependent perturbation theory

Time-evolution operator:

$$\Psi(t) = \boldsymbol{U(t,t_0)}\Psi(t_0)$$

$$\boldsymbol{U(t,t_0)} \;=\; 1 + \sum_{n=1}^{\infty} \frac{(-\mathrm{i})^n}{n!} \int_{t_0}^{t} \mathrm{d}^4 x_n \ldots \int_{t_0}^{t} \mathrm{d}^4 x_1 \, T_{\mathrm{D}}\Big[\mathcal{H}'_{\mathrm{I}}(x_n) \ldots \mathcal{H}'_{\mathrm{I}}(x_1)\Big]$$

$\mathcal{H}'_{\mathrm{I}}(x)$ the perturbation density in Interaction Picture

Adiabatic damping:

$$\mathcal{H}'_{\mathrm{I}}(x) \Rightarrow \mathcal{H}'_{\mathrm{I}}(x)\, e^{-\gamma|t|} \qquad \boldsymbol{U(t,t_0)} \Rightarrow \boldsymbol{U_{\gamma}(t,t_0)} \qquad \Psi(t) \to \Psi_{\gamma}(t)$$

$$\Psi_0 = \lim_{t \to -\infty} \Psi_{\gamma}(t)$$

$U(\infty, -\infty) = S$ is the $S - matrix$

but we shall consider **finite** final times:

$$U(t, -\infty)$$

Gell-Mann–Low theorem

Time-independent wave function given by

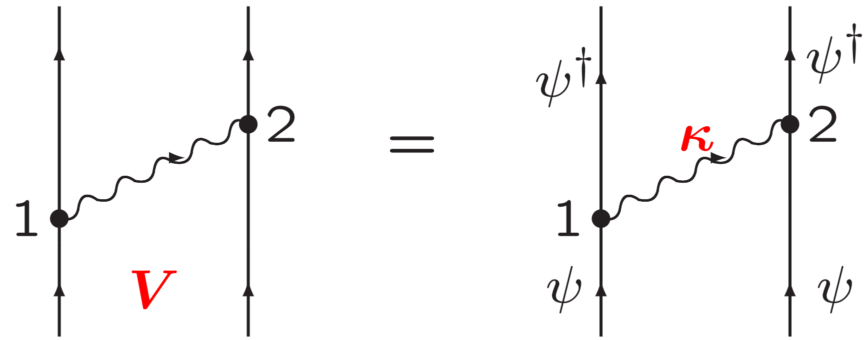
$$\Psi = \lim_{\gamma \to 0} \frac{U_\gamma(0, -\infty)\big|\Psi_0\big\rangle}{\langle \Psi_0 | U_\gamma(0, -\infty)\,|\Psi_0\rangle}$$

$\big|\Psi_0\big\rangle = P\Psi$ unperturbed wave function

The evolution operator **singular** as $\gamma \to 0$

The denominator cancels the singularities

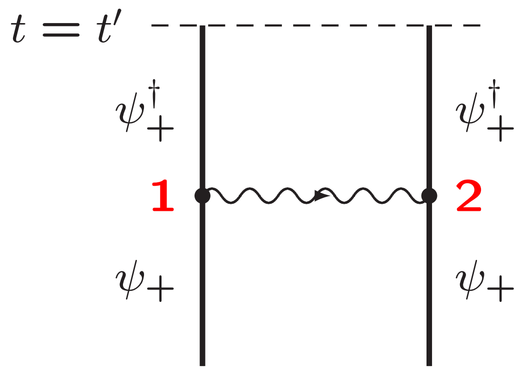
Brueckner-Goldstone Linked-Diagram Theorem



Effective-potential operator $(\boldsymbol{V})$
$=$ **Interaction kernel** $(\boldsymbol{\kappa})$
$+$ **el. field operators** $(\psi^\dagger, \psi)$

$$\boldsymbol{V}(\boldsymbol{t_1}, \boldsymbol{t_2}) = \frac{1}{2} \iint \mathrm{d}^3\boldsymbol{x}_1 \mathrm{d}^3\boldsymbol{x}_2 \, \psi^\dagger(x_1)\psi^\dagger(x_2) \, \boldsymbol{\kappa}(\boldsymbol{x_1}, \boldsymbol{x_2}) \, \psi(x_2)\psi(x_1)$$

Evolution operator for first-order interaction



$$U^{(2)}(t',-\infty) = -\iint_{-\infty}^{t'} \mathrm{d}t_1\,\mathrm{d}t_2\, V(t_1,t_2)\, \mathrm{e}^{-\gamma(|t_1|+|t_2|)}$$

Single-photon exchange

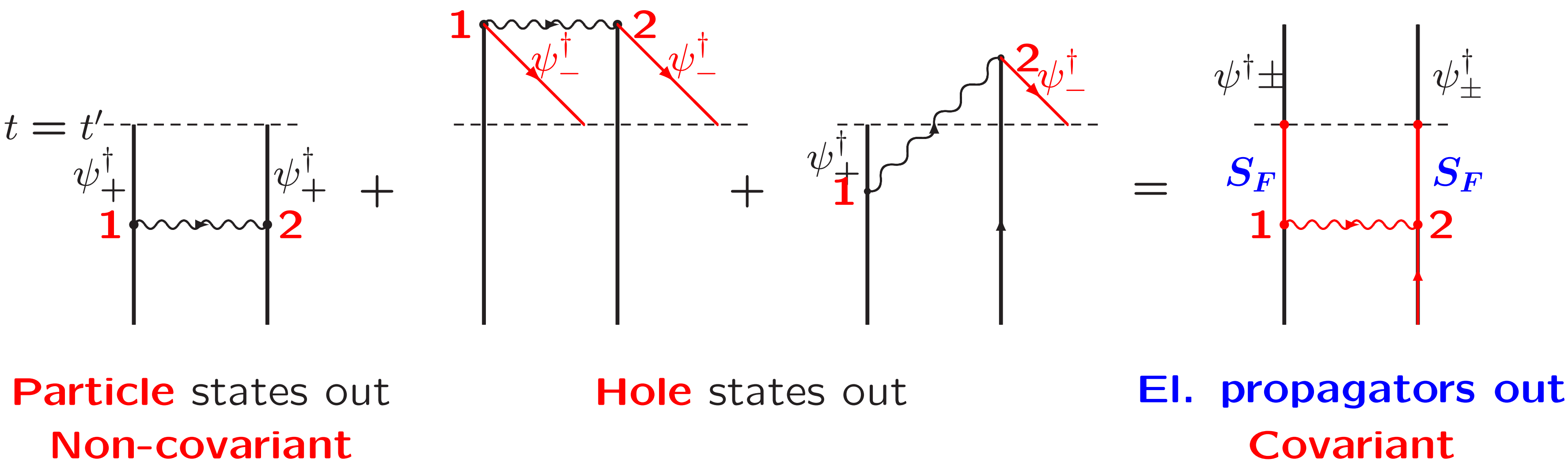
$$\kappa(x_1,x_2) = \alpha_1^{\mu}\,\mathrm{i}\,\underbrace{D_{\mathrm{F}\mu\nu}(x_2-x_1)}_{\text{Photon propagator}}\,\alpha_2^{\nu}$$

t_1 and t_2 integrated only from $-\infty$ to t'.

Non-covariant

Covariant evolution operator

Phys. Rev. A **64**, 062505 (2001); Physics Reports **Jan 2004**;



$$U^{(2)}_{\rm Cov}(t',-\infty) = -\iint \mathrm{d}^3\boldsymbol{x}'_1 \mathrm{d}^3\boldsymbol{x}'_2\;\psi^\dagger(x'_1)\psi^\dagger(x'_2)\;\psi(x'_1)\psi(x'_2)\iint_{-\infty}^{\infty}\mathrm{d}t_1\,\mathrm{d}t_2\,V(t_1,t_2)\,\mathrm{e}^{-\gamma(|t_1|+|t_2|)}$$

t_1 **and** t_2 **integrated over all times**

The evolution operator is singular in higher orders

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

Reduced evolution operator is regular

Factorization theorem for $t = 0$:

$$U_\gamma(0,-\infty)P = \underbrace{\left[1 + Q\,\widetilde{U}_\gamma(0,-\infty)\right]}_{\text{Regular}}\, \underbrace{P\, U_\gamma(0,-\infty)}_{\text{Singular}}\, P$$

Insert factorization theorem

$$U_\gamma(0,-\infty)P = \left[1 + Q\,\widetilde{U}_\gamma(0,-\infty)\right] P\,U_\gamma(0,-\infty)P$$

into Gell-Mann–Low formula:

$$\Psi = \frac{U_\gamma(0,-\infty)\left|\Psi_0\right\rangle}{\langle\Psi_0|U_\gamma(0,-\infty)\,|\Psi_0\rangle}$$

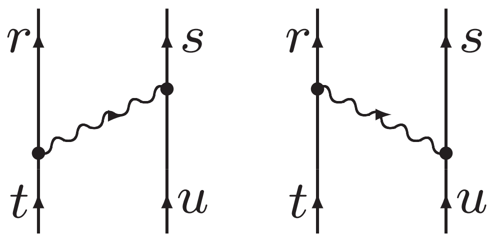
$$\Psi = \underbrace{\left[1 + Q\,\widetilde{U}_\gamma(0,-\infty)\right]}_{\text{Wave Op: }\Omega}\; P\underbrace{\frac{U_\gamma(0,-\infty)|\Psi_0\rangle}{\langle\Psi_0|U_\gamma(0,-\infty)\,|\Psi_0\rangle}}_{\text{Model fcn: }\Psi_0 = P\Psi}$$

Wave Op: Ω Model fcn: $\Psi_0 = P\Psi$

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

Wave operator for energy-dependent interactions

First-order interaction



$$\Omega^{(1)}(E_0) = Q\widetilde{U}^{(2)}(0) = \frac{Q}{E_0 - H_0} V(E_0)$$

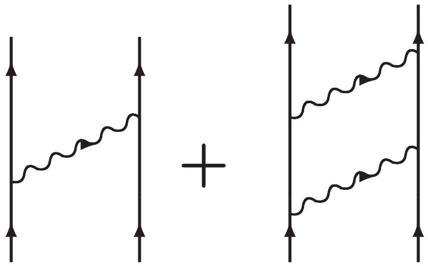
when operating on a state of energy E_0

$$\Big\langle rs \Big| V(z) \Big| tu \Big\rangle = \int \frac{\mathrm{d}z}{2\pi} \langle rs|\kappa(z)|ab\rangle \Big[\frac{1}{E_0 - \varepsilon_r - \varepsilon_u - z} + \frac{1}{E_0 - \varepsilon_t - \varepsilon_s + z}\Big]$$

First-order effective Hamiltonian

$$H_{\text{eff}}^{(1)} = PV(E_0)P$$

Second-order interaction



$$\Omega^{(1)}(E_0) = Q\widetilde{U}^{(2)}(0) = \frac{Q}{E_0-H_0}V(E_0)$$

$$\Omega^{(2)}(E_0) = \frac{Q}{E_0-H_0}V(E_0)\,\Omega^{(1)} + \boxed{\Big(\frac{\partial\Omega^{(1)}}{\partial\mathcal{E}}\Big)_{E_0} H_{\text{eff}}^{(1)}}$$

Last term represents model-space contributions

$$\Big(\frac{\partial\Omega^{(1)}}{\partial\mathcal{E}}\Big)_{E_0} = -\frac{Q}{E_0-H_0}\Omega^{(1)} + \frac{Q}{E_0-H_0}\Big(\frac{\partial V}{\partial\mathcal{E}}\Big)_{E_0}$$

folded diagrams and **potential derivatives**
MBPT S-matrix (ref.state.contr.)

Energy-independent interaction:

$$\Omega^{(2)} = \frac{Q}{E_0-H_0}V\Omega^{(1)} - \frac{Q}{E_0-H_0}\Omega^{(1)}H_{\text{eff}}^{(1)}$$

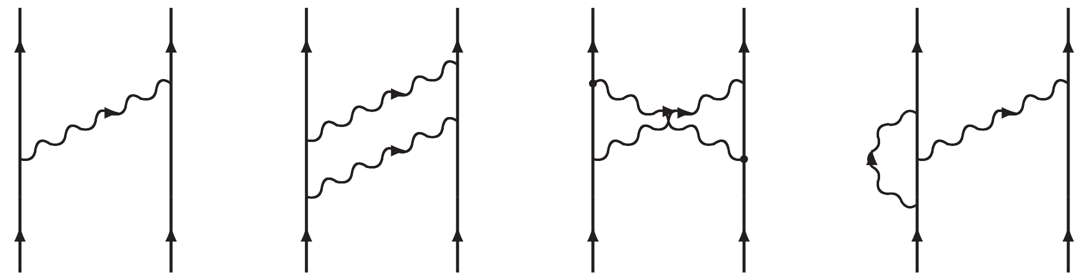
$$\big(E_0-H_0\big)\,\Omega^{(2)} = Q\,V\Omega^{(1)} - \Omega^{(1)}H_{\text{eff}}^{(1)}$$

folded

Std Rayleigh-Schrödinger expansion

Generalized effective-potential

We consider all **irreducible** interaction potential operators

$\mathcal{V}(E_0) =$  $\cdots$

All-order RS expansion for energy-dep. interactions:

$$\boxed{\Omega(E_0) = \bar{\Omega}(E_0) + \sum \frac{1}{n!} \left(\frac{\partial^n \bar{\Omega}}{\partial \mathcal{E}^n}\right)_{E_0} (H'_{\text{eff}})^n}$$

$$\bar{\Omega}(E_0) = 1 + \Gamma_Q(E_0)\mathcal{V} + \Gamma_Q(E_0)\mathcal{V}\,\Gamma_Q(E_0)\mathcal{V} + \cdots$$

$$\Gamma_Q(E_0) = \frac{Q}{E_0 - H_0}$$

Recursive **Bloch** form:

$$Q\Omega = \Gamma_Q(E_0)\mathcal{V}\,\Omega + \left(\frac{\partial\Omega}{\partial\mathcal{E}}\right)^*_{E_0} H'_{\text{eff}}$$

Unlinked diagrams eliminated in each order

Linked-diagram expansion:

$$Q\Omega = \left[\Gamma_Q(E_0)\mathcal{V}\,\Omega + \left(\frac{\partial\Omega}{\partial\mathcal{E}}\right)^*_{E_0} H'_{\text{eff}}\right]_{\text{linked}}$$

Energy-independence:

$$Q\Omega = \Gamma_Q V\,\Omega - \Gamma_Q\Omega\,H'_{\text{eff}}$$

$$(E_0 - H_0)\Omega = V\,\Omega - \Omega\,H'_{\text{eff}}$$

which is the standard Bloch equation

Connection to Bethe-Salpeter eqn

Start with Rayleigh-Schrödinger expansion:

$$\Omega(E_0) = \bar{\Omega}(E_0) + \sum \frac{1}{n!} \left(\frac{\partial^n \bar{\Omega}}{\partial \mathcal{E}^n} \right)_{E_0} (H'_{\text{eff}})^n$$

Operate on model function:

$$\Omega(E_0)|\Psi_0\rangle = \bar{\Omega}(E_0)|\Psi_0\rangle + \sum \frac{1}{n!} \left(\frac{\partial^n \bar{\Omega}}{\partial \mathcal{E}^n} \right)_{E_0} (\Delta E)^n |\Psi_0\rangle = \bar{\Omega}(E)|\Psi_0\rangle$$

Taylor expansion

Shifts the energy parameter of $\bar{\Omega}$ from E_0 to $E_0 + \Delta E = E$

Yields the Brillouin-Wigner expansion

$$\bar{\Omega}(E)|\Psi_0\rangle = \left[1 + \frac{Q}{E - H_0} \mathcal{V}(E) + \frac{Q}{E - H_0} \mathcal{V}(E) \frac{Q}{E - H_0} \mathcal{V}(E) + \cdots \right] |\Psi_0\rangle$$

Identity holds only in infinite order

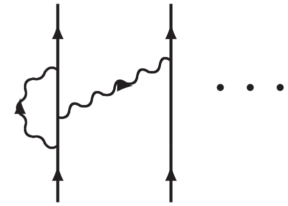
BW expansion:

$$|\Psi\rangle = |\Psi_0\rangle + \frac{Q}{E - H_0}\,\mathcal{V}(E)\,|\Psi\rangle$$

$$(E - H_0)\,Q|\Psi\rangle = Q\mathcal{V}(E)\,|\Psi\rangle$$

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

Bethe-Salpeter equation in Schrödinger-like form

$$\mathcal{V} =$$ 

Quasi-degenerate case:

$$\boxed{\left[\Omega, H_0\right] P = \mathcal{V}(E)\,\Omega P - \Omega P\,\mathcal{V}(E)\,\Omega P}$$

Bethe-Salpeter-Bloch equation

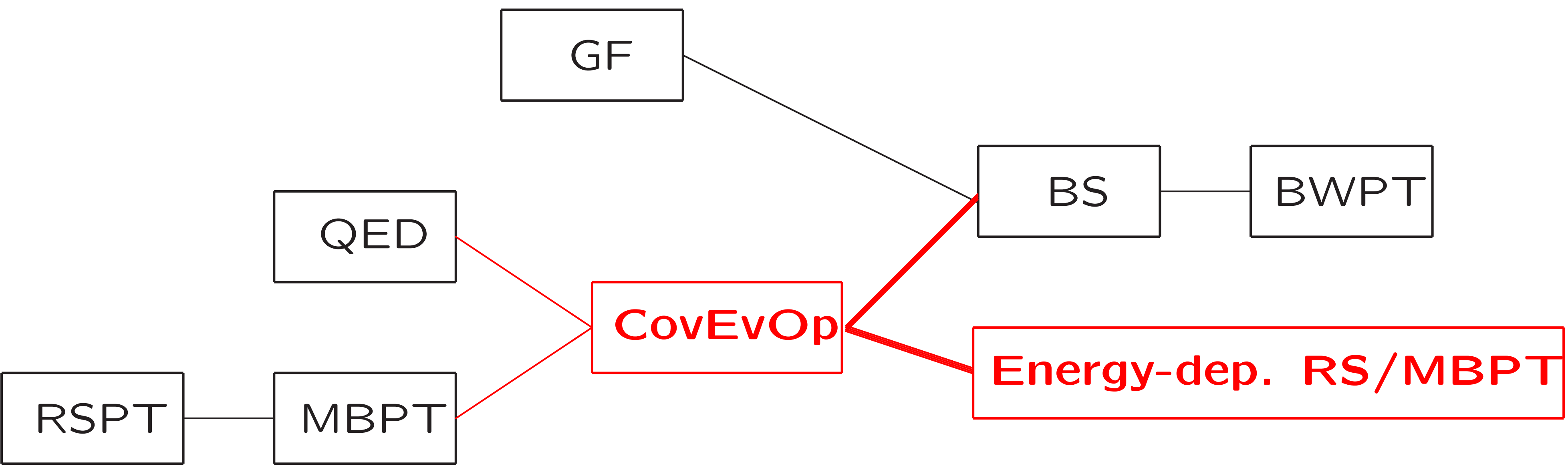
Compare energy-independent MBPT:

$$\left[\Omega, H_0\right] P = V\Omega P - \Omega\,P V \Omega\,P$$

Generalized MBPT

Connection with Bethe-Salpeter Eq.

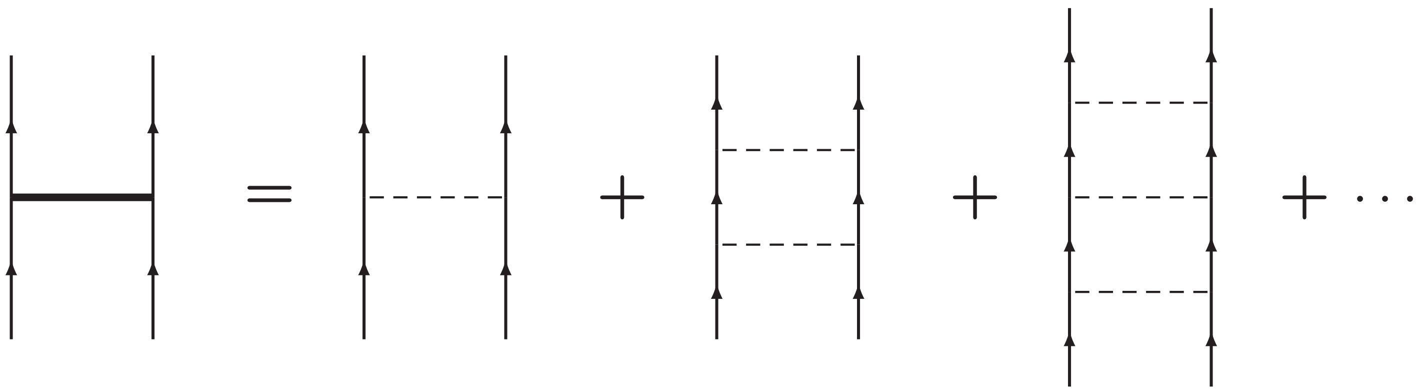
Einstein Centennial Review Paper: Can. J. Physics, March 2005



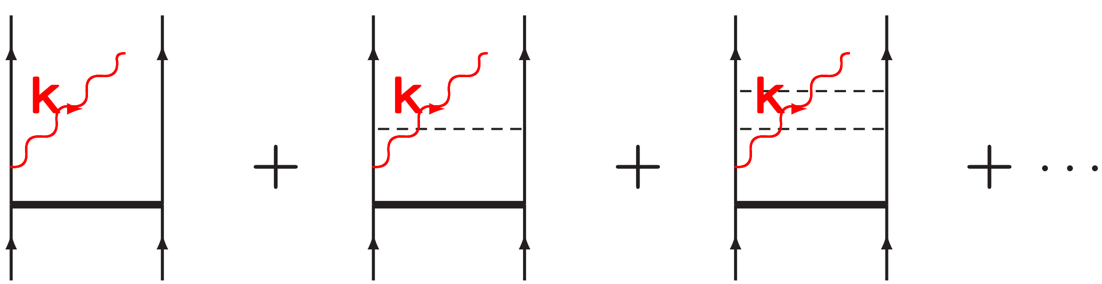
Numerical solution

Sten Salomonson and Daniel Hedendahl

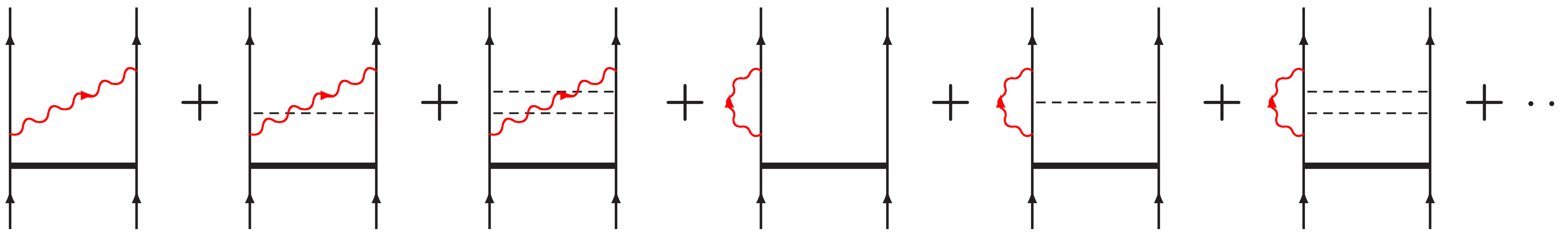
Relativistic pair function



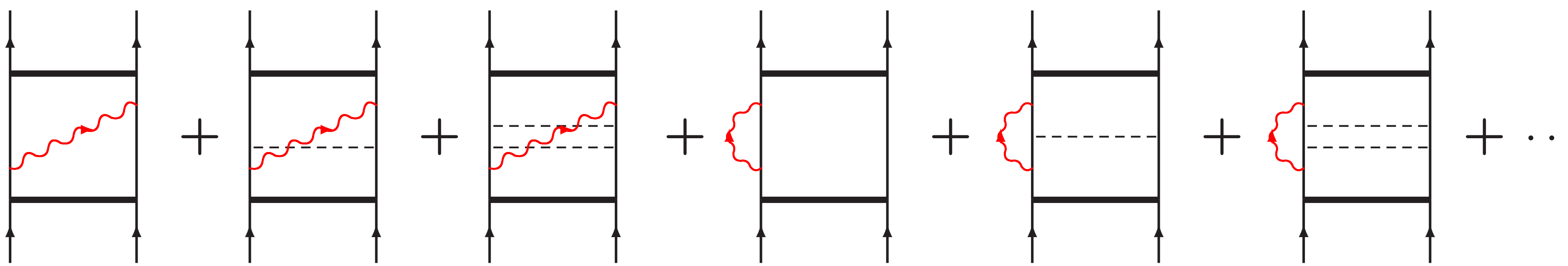
with an uncontracted photon



Absorb the photon and integrate over momentum



Pair functions iterated further



QED effects evaluated with correlated wave functions

Summary and Conclusions

1. A Covariant-evolution-operator method has been developed capable of handling quasi-degeneracy for energy-dependent interactions (QED)
(Demonstrated with energy of $^3P_1$ state of He-like ions)

2. Further development leads to
generalized Rayleigh-Schrödinger perturbation expansion
for energy-dependent perturbations

3. Represents a merger of MBPT and QED

4. Numerical procedure being deveoped
will be applied to the fs of light He-like ions