Field-Theoretical Approach to Many-Body Perturbation Theory: Combining MBPT and QED

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Abstract. Many-Body Perturbation Theory (MBPT) is today highly developed. The electron correlation of atomic and molecular systems can be evaluated to essentially all orders of perturbation theory—also relativistically (RMBPT)—by means of techniques of Coupled-Cluster type. When high accuracy is needed, effects beyond RMBPT will enter, i.e., effects of retarded Breit interaction and of radiative effects (Lamb shift), effects normally referred to as QED effects. These effects can be evaluated by means of special techniques, like S-matrix formulation, which cannot simultaneously treat electron correlation. It would for many applications be desirable to have access to a numerical technique, where effects of electron correlation and of QED could be treated on the same footing. Such a technique is presently being developed and gradually implemented at our laboratory. Some numerical results will be given.

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Introduction

Many-Body Perturbation Theory (MBPT) can effectively treat electron correlation of atomic and molecular systems to essentially all orders, using methods of Coupled-Cluster type [**?**], and it can also handle quasi-degeneracy problems using the "extended model-space technique" [**?**]. Quantum-electrodynamical (QED) effects, however, can be combined with standard MBPT only in the form of first-order energy corrections [**?**]. QED effects alone can be treated with higher accuracy, using S-matrix formulation or related numerical techniques [**?**], but these techniques cannot treat the electron correlation beyond second order. It would be desirable to have access to a technique capable of treating QED and electron correlation in a unified fashion. The Covariant-Evolution Operator technique, recently introduced at our laboratory for QED calculations [**? ? ?**], has such a potential that is presently being explored.

The covariant evolution operator represents the time evolution of the relativistic state vector. This operator contains singularities in the form of unlinked diagrams or intermediate model-space states, and eliminating these leads to what we refer to as the *Green's operator*. This operator, which plays a central role in the new formulation, is quite analogous to the Green's function of field theory and at the same time closely related to operators of many-body perturbation theory. Therefore, it serves as a link between field theory and MBPT and makes it possible to treat quantum-electrodynamics systematically within the framework of MBPT. For two-electron systems, treated to all orders, the procedure leads to the *Bethe-Salpeter equation*. The technique is presently being applied to light heliumlike ions, where quasi-degeneracy appears in excited states and where effects of electron correlation as well as of QED might be important. Presently, no other numerical technique is available for such calculations.

Basic formalism

In standard time-independent MBPT a number of target states are considered, satisfying the Schrödinger equation $H|\Psi^\alpha\rangle = E^\alpha|\Psi^\alpha\rangle$. The basic tools are the wave operator $\hat{\Omega}$, which transforms the model states to the full target states, and the effective Hamiltonian $H_{\rm eff}$, which operating on a model state yields the corresponding exact energy [**?**]

$$|\Psi^\alpha\rangle = \hat{\Omega}|\Psi_0^\alpha\rangle; \qquad \hat{H}_{\rm eff}|\Psi_0^\alpha\rangle = E^\alpha|\Psi_0^\alpha\rangle \tag{1}$$

The model states are the projections of the target states on the model space (intermediate normalization) $|\Psi_0^\alpha\rangle = P|\Psi^\alpha\rangle$. The wave operator satisfies the *generalized Bloch equation* in the linked-diagram form

$$\big[\hat{\Omega}, H_0\big]P = Q\big(V\hat{\Omega} - \hat{\Omega}V_{\rm eff}\big)_{\rm linked}P \tag{2}$$

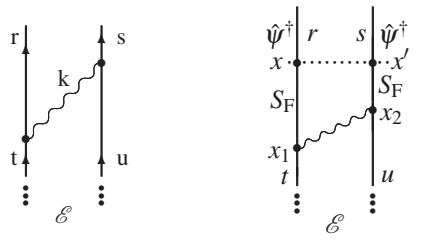

FIGURE 1. The non-covariant and the covariant evolution-operators for single-photon exchange. In the covariant form (right) the outgoing lines can be particle or hole lines.

with $Q = 1 - P$; $H = H_0 + V$ and $H_{\text{eff}} = PH_0P + V_{\text{eff}}$ with V_{eff} being the effective interaction. The Bloch equation generates the linked-diagram expansion, valid also in the quasi-degenerate case. The last term ($\hat{\Omega}V_{\text{eff}}$) gives rise to "folded" diagrams.

The normal-ordered exponential Ansatz, $\hat{\Omega} = \{e^S\}$, yields the corresponding *Coupled-Cluster Approach*

$$\big[S_n, H_0\big]P = Q\big(V\hat{\Omega} - \hat{\Omega}V_{\text{eff}}\big)_{\text{conn},n}P \tag{3}$$

with the cluster operator separated into one-, two-,...body parts, $S = S_1 + S_2 + \cdots$. The second term, S_2, represents the important *pair correlation*. The S diagrams are "connected", which is distinct from "linked" diagrams [**?**].

In time-dependent perturbation theory the basic tool is the *time-evolution operator*, in the interaction picture defined

$$|\Psi(t)\rangle = \hat{U}(t,t_0)\,|\Psi(t_0)\rangle \qquad (t > t_0) \tag{4}$$

leading to the expansion

$$\hat{U}(t,t_0) = \sum_{n=0}^{\infty} \frac{(-\mathrm{i})^n}{n!} \int_{t_0}^{t} \mathrm{d}x_1^4 \ldots \int_{t_0}^{t} \mathrm{d}x_n^4\, T\big[\hat{H}'(x_1)\ldots\hat{H}'(x_n)\big] \tag{5}$$

T is the time-ordering operator and $\hat{H}'(x) = -e\hat{\psi}^\dagger\alpha^\mu A_\mu\hat{\psi}$ represents the electron interaction with the electromagnetic field A_μ. The contraction of two such interactions corresponds to the exchange of a single retarded photon. The operator (**??**) is non-covariant, since time moves only in the positive direction (Fig. **??** left). It can be made covariant by inserting electron propagators on the in- and outgoing lines. Normally, we shall operate to the right on unperturbed model states, which implies that we can with adiabatic damping set the initial time $t_0 = -\infty$, and no propagators on incoming lines are needed. Time can then flow in both directions on outgoing lines (Fig. **??** right). We then express the covariant evolution operator for single-photon exchange

$$\hat{U}_{\text{Cov}}(t,-\infty) = \mathrm{i}^2 \iint \mathrm{d}^3x\,\mathrm{d}^3x'\,\hat{\psi}^\dagger(x)\hat{\psi}^\dagger(x') \iint \mathrm{d}^4x_1\,\mathrm{d}^4x_2\,S_{\text{F}}(x,x_1)S_{\text{F}}(x',x_2)V_{\text{sp}}(x_1,x_2)\,\hat{\psi}(x_2)\hat{\psi}(x_1) \tag{6}$$

where the energy-dependent potential is in the Fourier transform given by

$$\langle rs|V_{\text{sp}}(\mathscr{E})|ab\rangle = \left\langle rs\right| \int_0^\infty \mathrm{d}k\, f(k) \left[\frac{1}{\mathscr{E} - \varepsilon_r - \varepsilon_u - (k - \mathrm{i}\gamma)_r} + \frac{1}{\mathscr{E} - \varepsilon_s - \varepsilon_t - (k - \mathrm{i}\gamma)_s}\right] \left|tu\right\rangle \tag{7}$$

ε_x is the energy of the orbital x, generated by the Dirac equation in the nuclear field; $(\cdot)_x$ has the same sign as ε_x; k is the photon momentum and $f(k)$ is a gauge-dependent function. This expression is valid also when energy is not conserved between initial and final states. This is needed for treating quasi-degeneracy with the extended-model-space technique [**?**]. In the case of energy conservation, $q + q' = 0$, (**??**) goes over into standard S-matrix result [**?**].

Generally, the covariant evolution operator is singular, due to intermediate model-space-states. Eliminating the singularities, leads to what we refer to as the *Green's operator*, $\hat{G}$. This is very closely related to the field-theoretical Green's function, the main difference being that it is an operator, while the Green's function is a function. The Green's operator is separated into open and closed parts, $\hat{G} = 1 + \hat{G}_{\text{op}} + \hat{G}_{\text{cl}}$, where $\hat{G}_{\text{op}}$ operates outside and $\hat{G}_{\text{cl}}$ inside the model space. The former is essentially the MBPT wave operator and the latter yields the effective interaction (**??**, **??**)

$$\hat{\Omega} = 1 + \hat{G}_{\text{op}}\,; \qquad V_{\text{eff}} = P\Big(\mathrm{i}\frac{\partial}{\partial t}\,\hat{G}_{\text{cl}}(t)\Big)_{t=0}P \tag{8}$$

The Green's operator can be applied also to energy-dependent interactions of QED type and therefore forms a link between MBPT and quantum field theory.

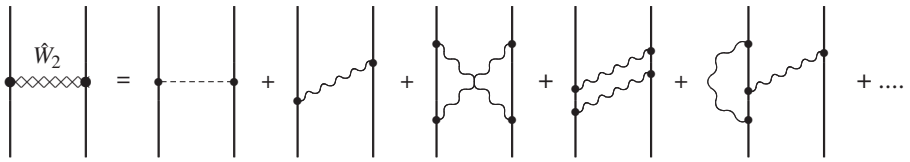

FIGURE 2. The two-body part of the effective potential $\hat{W}$ in the Bethe-Salpeter equation (**??**) contains all irreducible two-body potential diagrams, including the Coulomb interaction as well as all retardation and radiative effects.

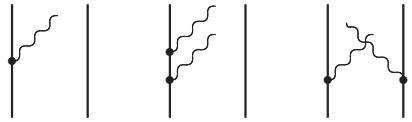

FIGURE 3. The wave function with uncontracted photons lies in an extended Fock space.

Eliminating singularities from the covariant evolution operator, leaves some finite residuals [**? ?**],

$$\hat{G}(t) = \hat{G}_0(t) + \sum_{n=1}^{\infty} \frac{\delta^n \hat{G}_0(t)}{\delta \mathscr{E}^n} \left(\hat{V}_{\rm eff}\right)^n \tag{9}$$

where $\hat{G}_0(t)$ represents the Green's operator without any intermediate model-space states

$$\hat{G}_0 = 1 + \Gamma_Q \hat{W} + \Gamma_Q \hat{W} \Gamma_Q \hat{W} + \cdots ; \qquad \Gamma_Q = \frac{Q}{E_0 - H_0} \tag{10}$$

and $\hat{W}$ represents all irreducible multi-photon interactions (Fig. **??**). The difference ratios go over into derivatives in the case of complete degeneracy. These terms represent the model-space contributions and are analogous to the folded diagrams of open-shell MBPT (**??**), but contain also energy derivatives (difference ratios) of the energy-dependent interaction. Summing the contributions to all orders is in the single-reference case equivalent to the full *Bethe-Salpeter (BS) equation*

$$\boxed{(E - \hat{H}_0)|\Psi\rangle = \hat{W}(E)|\Psi\rangle} \tag{11}$$

This equation can be solved self-consistently, using e.g. Brillouin-Wigner perturbation theory. For many-body purposes (size-extensivity etc. [**?**]) we would prefer to work with the Rayleigh-Schrödinger theory and the linked-diagram representation, as in standard MBPT. This can be achieved by transforming the BS equation to the corresponding Bloch equation (**??**)

$$\boxed{(E_0 - \hat{H}_0)\,\hat{\Omega}P = \left(\hat{W}(E)\,\hat{\Omega} - \hat{\Omega}\hat{W}_{\rm eff}(E)\right)_{\rm linked} P} \tag{12}$$

referred to as the *Bethe-Salpeter-Bloch equation*. Note that the energy parameter of the BS potential $\hat{W}$ and of the BS effective interaction $\hat{W}_{\rm eff} = P\hat{W}\hat{\Omega}P$ is the target-state energy E, and not the model-state energy E_0, as one might first have expected. This shift is due to the derivative terms of the expansion (**??**). The Bloch equation (**??**) can be used to generate a perturbative expansion of the wave operator for energy-dependent interactions. The difficulty is here to evaluate the energy derivatives of the (multi-photon) perturbation ($\hat{W}$). This difficulty can be overcome by working in the extended Fock space.

Implementation. Fock space treatment

With uncontracted interactions (**??**) the wave function lies in an extended Fock space with a variable number of (virtual) photons (Fig. **??**). This is utilized for the numerical evaluation. Here, the Bloch equation (**??**) has a particularly simple structure

$$\left[\hat{\Omega}, H_0\right] P = \left(\hat{H}'\hat{\Omega} - \hat{\Omega} V_{\rm eff}\right)_{\rm linked} P \tag{13}$$

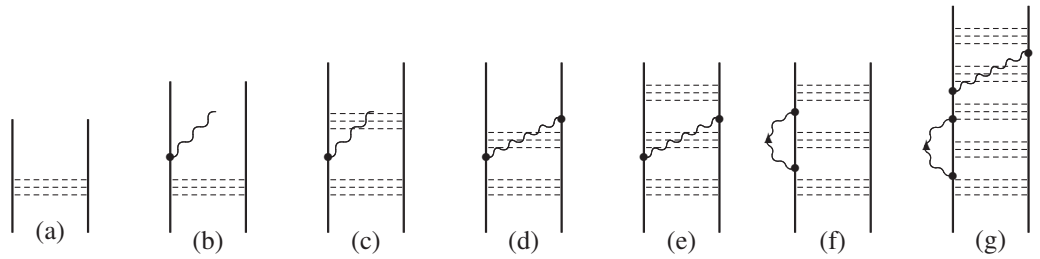

FIGURE 4. Lowest-order contribution to the wave operator in the extended Fock space and the corresponding contribution to the single- and double- photon exchange.

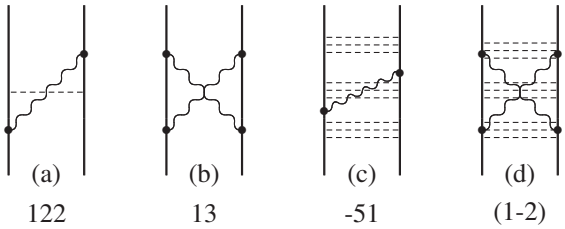

FIGURE 5. Numerical results for non-radiative QED contributions (retarded interactions) in the ground state of He-like neon (in μ Hartree).

where $\hat{H}'$ is the energy-independent perturbation (**??**) and $V_{\text{eff}} = PH'\hat{\Omega}P$. The energy dependence is here introduced by the energy denominator, and the energy derivative by the folded diagrams with a double energy denominator. The energy-dependent interaction can be mixed with energy-independent Coulomb interactions.

Starting with iterating the Coulomb interaction, leads to the standard (relativistic) pair-correlation (S_2) function (Fig. **??** a). We then generate a new pair function with one uncontracted photon (b), and additional Coulomb interactions can be added before and after closing the photon (c-e). This leads to one *retarded Breit interaction* with a number of Coulomb interactions. Absorbing the photon on the same electron, leads instead to *electron self energy and vertex corrections*—after proper renormalization (f). The whole procedure can then be repeated (g). In principle, it is possible to create a second photon, before the first in absorbed (Fig. **??**), which would generate irreducible multi-retarded photon exchange. This, however, would exceed the computing power we presently have available. The effect might be estimated analytically, though.

Some numerical results for heliumlike neon are shown in Fig. **??**. The first two diagrams (a,b) can be evaluated by means of standard QED techniques, like S-matrix formulation [**?**]. Diagrams of type (c), which represent first-order QED effects with high-order electron correlation, have never been numerically evaluated before. It is interesting to note that this effect dominates heavily over the second-order QED effect (b). This demonstrates clearly the importance of combining QED with electron correlation in a systematic fashion, not only for the lightest systems.

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