Virtual-pair effects in atomic structure theory

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A modified perturbation procedure for computing relativistic atomic bound-state energies is described, in which the instantaneous Coulomb interaction is included in the unperturbed QED Hamiltonian and the effect of virtual electron-positron pairs and of virtual transverse photons is treated as the perturbation. To illustrate the method in the context of a simple model, a one-electron atom is considered and a "one-pair" approximation is analyzed in detail. The approach is based on the resolvent-operator formulation of many-body time-independent perturbation theory. The removal of divergent vacuum-to-vacuum matrix elements is easily accomplished in this formulation, and it leads rather directly to the derivation of a modified Dirac equation in which all perturbative effects are contained in an effective one-electron potential. A set of integral equations for the evaluation of the effective potential in the one-pair model is derived. These equations have the same structure as the Dyson-Schwinger equations of covariant QED and serve a similar purpose. That is, they allow for the isolation of the divergent self-energy and vertex parts, leaving a finite kernel (the K matrix) which contains the effects of multiparticle intermediate states. In the one-pair model considered here the intermediate states consist of an electron and a virtual pair interacting Coulombically. It is shown that the K matrix can be constructed with the aid of a rigorous minimum principle of the Rayleigh-Ritz type. That such a minimum principle exists appears to be an advantage of the noncovariant Hamiltonian procedure. The inapplicability of standard renormalization methods is, however, a distinct disadvantage. While some progress (the removal of vacuum divergences and the isolation of divergent parts in the integral equation) is reported, a full resolution of the renormalization problem in the Hamiltonian formulation remains to be developed.

I. INTRODUCTION

In recent years there has been an increasing awareness of the need for improved accuracy in the computation of atomic bound-state energies and wave functions with relativistic effects accounted for. While the standard Hartree-Fock-Dirac procedure provides satisfactory results in many cases of interest, there are circumstances in which alternative formulations might play a useful role; one would look for methods which would allow, in principle, the efficient and systematic improvement of the calculational accuracy. Quantum electrodynamics, in the time-independent formulation, provides a proper foundation for the theory, as has been emphasized.[1,2] A possible practical advantage of this approach is that it may be possible to borrow techniques developed over the years for nonrelativistic calculations—for example, the use of the Rayleigh-Ritz minimum principle in the treatment of multiparticle Coulomb interactions—and apply them effectively to relativistic problems. The absence of time variables is a simplifying feature, and this can be especially important in dealing with multielectron atoms. One pays the price for this, of course, in the loss of manifest covariance, which complicates the problem of removing divergences in a systematic and physically consistent manner.

It is convenient, in the time-independent formulation of QED, to express the total Hamiltonian as the sum of a "no-pair" component, which includes the instantaneous Coulomb interaction between electrons but does not allow for virtual-photon or pair creation, and a remainder taken as the perturbation.[2] There are no formal difficulties associated with the eigenvalue problem based on the no-pair Hamiltonian. Since the spectrum is bounded from below, the Rayleigh-Ritz principle can be used to find approximate solutions without the occurrence of "variational collapse" in the minimization procedure.[3] Furthermore, in the absence of self-energy effects the divergence difficulty does not arise at this level of approximation. Solutions of the no-pair model will provide energies and wave functions which should prove to be accurate enough for many applications. (Such solutions would include correlation effects not contained in the Hartree-Fock-Dirac approximation.)

In order to establish the validity of the no-pair model, or improve on it when necessary, one must examine higher-order terms in the perturbation expansion which, as mentioned, represent the effect of the virtual creation and annihilation of transverse photons and of electron-positron pairs. Several specific calculations, based on the no-pair model and corrections to it, have been performed.[4–6] The main focus of the present discussion will be on the formulation of variational methods to carry out sums over intermediate states. (The utility of such methods was demonstrated some time ago in connection with a Lamb-shift calculation in helium.[7]) A complete analysis of the renormalization problem in the noncovariant Hamiltonian formulation of QED has not yet been given and no attempt will be made to provide one here.

Nevertheless, we are obliged to include some discussion of divergences in order to verify the validity of the minimum principle in the evaluation of higher-order perturbation terms. In an infinite subset of such terms one encounters sums over intermediate states corresponding to a system differing from that of the no-pair model by the presence of an additional electron-positron pair. The minimum principle is not directly applicable in this one-pair sector since the pair can virtually annihilate itself and then be recreated, and the matrix element for this process introduces a divergent photon self-energy integral. (It is, of course, just the divergence problem which prevents one from applying the minimum principle directly to the expectation value of the Hamiltonian.) In Sec. III A we outline the procedure whereby these divergent contributions (and others associated with the vertex function) can be isolated. With these divergent parts removed the finite remainder satisfies the minimum principle, as shown in Sec. III B.

The modified perturbation theory is formulated in Sec. II A. The resolvent-operator method of many-body perturbation theory, developed by Hugenholtz,[8] is adopted for this purpose. This approach has the merit that it allows, in a straightforward way, for the removal of divergences associated with vacuum-to-vacuum transitions to all orders in the expansion. For the sake of orientation we have written out, in Sec. II B, the integral expressions which represent the second-order electron self-energy function for a one-electron atom. The calculation illustrates how noncovariant contributions involving Coulomb and transverse-photon interactions can be combined, resulting in a covariant and renormalizable expression. The divergent photon self-energy function in second order can be treated in a similar way. (Use of the Coulomb gauge is not an obstacle to renormalization.[9] An explicit demonstration of renormalization in the Coulomb gauge, for the second-order self-energy and vertex functions, has been provided recently by Adkins.[10])

In order to permit an analysis of pair effects in reasonably explicit form the discussion has been confined to the study of a one-electron atom, and contributions involving only a single virtual pair are considered. This is a relatively simple model. Even so, the treatment of the three-body intermediate states leading to a separation of divergent and nondivergent parts is fairly intricate. Methods developed previously for nonrelativistic three-body scattering problems, involving the use of an effective potential to describe the projectile-target interaction, turn out to be useful here. It is the effective potential, from which divergences have been removed, to which the minimum principle is applied. The integral equations introduced here are similar in form to the Dyson-Schwinger (DS) equations of covariant perturbation theory. The effective potential mentioned above has its analog in one of the "irreducible kernels" of the DS equations. These kernels have the well-known and important property of being *essentially* finite, in the sense that divergences appear only through the insertion of vertex and self-energy corrections. It is for this reason that the DS equations provide a convenient framework for renormalization and, more to the point in the present context, allow us to identify the matrix elements which are suitable for variational construction.

II. EFFECTIVE-HAMILTONIAN METHOD BASED ON THE RESOLVENT OPERATOR

A. Formulation

Consideration of the resolvent operator

$$R(z)=(z-H)^{-1} \tag{2.1}$$

provides a convenient starting point for the development of time-independent multiparticle perturbation theory.[8] Writing the QED Hamiltonian as $H=H_0+V$, and introducing the resolvent $R_0(z)=(z-H_0)^{-1}$ of the unperturbed system, we have the integral equation

$$R(z)=R_0(z)+R_0(z)VR(z)\ , \tag{2.2}$$

whose iterative solution generates the perturbation expansion. To simplify the discussion we confine our attention to a system consisting of a single electron bound in the Coulomb field of a fixed nucleus. The extension of the analysis to multielectron systems is straightforward in principle.

Let us consider the matrix element $\langle n'|R(z)|n\rangle$. Here $|n\rangle$ and $|n'\rangle$ represent eigenstates of H_0, corresponding to a single electron in the presence of the external field of the nucleus (but unperturbed by self-energy interactions) with positive-energy eigenvalues ε_n and $\varepsilon_{n'}$, respectively. Terms in the perturbation expansion of the matrix element can be represented by diagrams in the usual way. A connected diagram is one which cannot be separated into two distinct parts without breaking one or more of the internal propagator lines. Disconnected diagrams contain additional components representing vacuum-to-vacuum transitions which take place independently of the $n\rightarrow n'$ transition of interest. The matrix element $\langle n'|R(z)|n\rangle$ may be expressed, according to the Hugenholtz factorization theorem,[8] as the convolution of $\langle n'|\hat{R}(z)|n\rangle$, which is the sum of all connected terms, and $\langle 0|R(z)|0\rangle$ representing the sum of all vacuum components. This is written as

$$\langle n'|R(z)|n\rangle=\langle n'|\hat{R}(z)|n\rangle * \langle 0|R(z)|0\rangle\ , \tag{2.3}$$

where the convolution of two functions, say, $f(z)$ and $g(z)$, is defined as

$$f(z)*g(z)=\frac{1}{2\pi i}\int_c d\zeta\, f(z-\zeta)g(\zeta)\ ; \tag{2.4}$$

c is a counterclockwise contour enclosing the singularities of $g(z)$ on the real axis.

Consider now the sum of all terms contributing to the perturbation expansion of $\langle n'|\hat{R}(z)|n\rangle$ which do not contain any one-electron intermediate states. We write this sum as

$$(z-\varepsilon_{n'})^{-1}F_{n'n}(z)(z-\varepsilon_n)^{-1}\ ,$$

where we have used the relation $R_0(z)|n\rangle=(z-\varepsilon_n)^{-1}|n\rangle$ and have defined

$$F_{n'n}(z)=\langle n'|[V+VR_0(z)V+\cdots]'|n\rangle\ ; \tag{2.5}$$

the prime on the bracket enclosing the sum is to indicate that only connected diagrams are included in the perturbation expansion and no terms with one-electron intermediate states are retained. Since $\langle n'|\hat{R}|n\rangle$ is generated by stringing together the "one-electron irreducible" diagrams in all possible ways we have

$$\langle n'|\hat{R}(z)|n\rangle=\delta_{n'n}(z-\varepsilon_n)^{-1}+(z-\varepsilon_{n'})^{-1}\sum_{n''}^{(+)}F_{n'n''}(z)\langle n''|\hat{R}(z)|n\rangle\ . \tag{2.6}$$

A generalized sum is implied here, which includes an integration over continuum one-electron states in addition to a sum over discrete bound states. Only positive-energy states are included in the sum.

Suppose that $\langle n'|\hat{R}(z)|n\rangle$ has a pole at $\hat{E}_n$ with residue $\hat{\eta}_{n'n}$, and that $\langle 0|R(z)|0\rangle$ has a pole at E_0 with residue η_0. From the relation

$$\frac{a}{z-A}*\frac{b}{z-B}=\frac{ab}{z-A-B}\ , \tag{2.7}$$

it follows that $\langle n'|R(z)|n\rangle$ has a pole at $E_n\equiv E_0+\hat{E}_n$ with residue $\hat{\eta}_{n'n}\eta_0$. The state

$$|W_n\rangle=\eta_0^{-1}\lim_{z\to E_n}(z-E_n)R(z)|n\rangle \tag{2.8}$$

is an eigenstate of H with eigenvalue E_n, as is easily verified. The normalization has been chosen to ensure that its projection on state $\langle n'|$ can be expressed as

$$\langle n'|W_n\rangle=\lim_{z\to\hat{E}_n}(z-\hat{E}_n)\langle n'|\hat{R}(z)|n\rangle\ . \tag{2.9}$$

The energy $\hat{E}_n$, measured relative to the (divergent) vacuum self-energy, is the eigenvalue of physical interest.

Configuration-space representations of the preceding relations are obtained by introducing the wave function $\psi_n(\mathbf{x})=\langle\mathbf{x}|W_n\rangle$. Since the only one-electron components of $|W_n\rangle$ generated by the perturbation expansion are those with positive energy we may insert a positive-energy projection operator to obtain the expansion

$$\psi_n(\mathbf{x})=\sum_{n'}^{(+)}\langle\mathbf{x}|n'\rangle\langle n'|W_n\rangle=\sum_{n'}^{(+)}u_{n'}(\mathbf{x})\langle n'|W_n\rangle\ . \tag{2.10}$$

The spinors $u_n(\mathbf{x})$ satisfy the Dirac equation

$$h(\mathbf{x})u_n(\mathbf{x})=\varepsilon_n u_n(\mathbf{x}),\quad \varepsilon_n>0 \tag{2.11a}$$

where, with $\hbar=c=1$,

$$h(\mathbf{x})=\boldsymbol{\alpha}\cdot(-i\nabla)+\beta m+V_{\text{ext}}(\mathbf{x})\ . \tag{2.11b}$$

The negative-energy solutions, satisfying

$$h(\mathbf{x})v_m(\mathbf{x})=\varepsilon_m v_m(\mathbf{x}),\quad \varepsilon_m<0 \tag{2.11c}$$

will be needed later on. The orthonormality relations satisfied by these functions are[11]

$$\int u_{n'}^{\dagger}(\mathbf{x})u_n(\mathbf{x})d^3x=\delta_{n'n},\quad \int v_{m'}^{\dagger}(\mathbf{x})v_m(\mathbf{x})d^3x=\delta_{m'm}\ ,$$
$$\int v_m^{\dagger}(\mathbf{x})u_n(\mathbf{x})d^3x=\int u_n^{\dagger}(\mathbf{x})v_m(\mathbf{x})d^3x=0\ . \tag{2.12}$$

From Eq. (2.10) and the orthonormality property, we have

$$\int u_{n'}^{\dagger}(\mathbf{x})\psi_n(\mathbf{x})d^3x=\langle n'|W_n\rangle\ . \tag{2.13}$$

The function $\psi_n(\mathbf{x})$ satisfies a modified Dirac equation which incorporates self-energy effects. To derive this equation we use Eqs. (2.10) and (2.9) to write

$$[\hat{E}_n-h(\mathbf{x})]\psi_n(\mathbf{x})=\sum_{n'}^{(+)}u_{n'}(\mathbf{x})(\hat{E}_n-\varepsilon_{n'})\langle n'|W_n\rangle=\lim_{z\to\hat{E}_n}\sum_{n'}^{(+)}u_{n'}(\mathbf{x})(\hat{E}_n-\varepsilon_{n'})\times(z-\hat{E}_n)\langle n'|\hat{R}(z)|n\rangle\ . \tag{2.14}$$

From Eq. (2.6) we have

$$\lim_{z\to\hat{E}_n}(z-\hat{E}_n)(\hat{E}_n-\varepsilon_{n'})\langle n'|\hat{R}(z)|n\rangle=\sum_{n''}^{(+)}F_{n'n''}(\hat{E}_n)\langle n''|W_n\rangle\ . \tag{2.15}$$

Equation (2.14) then takes the form

$$[\hat{E}_n-h(\mathbf{x})]\psi_n(\mathbf{x})=\int M(\mathbf{x},\mathbf{x}';\hat{E}_n)\psi_n(\mathbf{x}')d^3x'\ , \tag{2.16}$$

where the effective potential is given by

$$M(\mathbf{x},\mathbf{x}';E)=\sum_{n'}^{(+)}\sum_{n''}^{(+)}u_{n'}(\mathbf{x})F_{n'n''}(E)u_{n''}^{\dagger}(\mathbf{x}')\ . \tag{2.17}$$

Since M is energy dependent the eigenvalue must be determined self-consistently from Eq. (2.16), a feature familiar from standard Brillouin-Wigner perturbation theory.

While we are studying a relatively simple one-electron problem, in which the negative-energy states correspond to positrons, it should be mentioned that very similar techniques could be applied to the study of a multielectron atom where, by suitable choice of Fermi energy level, the collection of negative-energy states is allowed to include, in addition to the positron degrees of freedom, occupied electronic levels. Renormalization effects associated with virtual excitation of occupied levels are finite and an analysis of higher-order corrections associated with virtual excitation of electron-hole pairs, along the lines given in the following, is immediately applicable.[12]

We recall here the form of the QED Hamiltonian. The unperturbed part $H_0=H_D+H_{\text{rad}}$ is the sum of the particle and radiation-field energy operators, which are expressed in terms of the field operators $\psi_D(\mathbf{x})$ and $\mathbf{A}(\mathbf{x})$. The particle field operator may be expanded as

$$\psi_D(\mathbf{x})=\sum_{n}^{(+)}A_n u_n(\mathbf{x})+\sum_{m}^{(-)}B_m^{\dagger}v_m(\mathbf{x})\ , \tag{2.18}$$

where A_n and B_m are electron and positron annihilation

operators with the property

$$A_n|0\rangle = B_m|0\rangle = 0 \ . \tag{2.19a}$$

The anticommutation relations are

$$\{A_{n'}, A_n^\dagger\} = \delta_{n'n}, \quad \{B_{m'}, B_m^\dagger\} = \delta_{m'm} \ , \tag{2.19b}$$

with all the other anticommutators vanishing. When put in normal-ordered form H_D becomes

$$H_D = \sum_n^{(+)} \varepsilon_n A_n^\dagger A_n + \sum_m^{(-)} |\varepsilon_m| B_m^\dagger B_m \ . \tag{2.20}$$

With the radiation field quantized in a box of volume L^3 the vector potential can be expanded as

$$\mathbf{A}(\mathbf{x}) = \sum_s (2k_s)^{-1/2} [a_s \mathbf{U}_s(\mathbf{x}) + a_s^\dagger \mathbf{U}_s^*(\mathbf{x})] \ , \tag{2.21}$$

where the index s specifies both the photon momentum $\mathbf{k}_s$ and the double-valued polarization index λ_s. The photon wave function is

$$\mathbf{U}_s(\mathbf{x}) = L^{-3/2} \mathbf{e}^{\lambda_s} \exp(i\mathbf{k}_s \cdot \mathbf{x}) \ , \tag{2.22}$$

with $\mathbf{k}_s \cdot \mathbf{e}^{\lambda_s} = 0$ in the Coulomb gauge adopted here. The relations

$$\begin{aligned} &a_s|0\rangle = 0 \ , \\ &[a_s, a_{s'}^\dagger] = \delta_{ss'}, \quad [a_s, a_{s'}] = [a_s^\dagger, a_{s'}^\dagger] = 0 \ , \end{aligned} \tag{2.23}$$

characterize the photon creation and annihilation operators. In its normal-ordered form the radiation-field energy is

$$H_{\text{rad}} = \sum_s k_s a_s^\dagger a_s \ . \tag{2.24}$$

The perturbation operator is $V = H_T + H_C$, with

$$H_T = e \int \psi_D^\dagger(\mathbf{x}) \boldsymbol{\alpha} \psi_D(\mathbf{x}) \cdot \mathbf{A}(\mathbf{x}) d^3x \tag{2.25}$$

representing the interaction with the transverse radiation field,[13] and

$$H_C = \tfrac{1}{2} \int \psi_D^\dagger(\mathbf{x}) \psi_D(\mathbf{x}) \frac{e^2}{4\pi|\mathbf{x}-\mathbf{x}'|} \psi_D^\dagger(\mathbf{x}') \psi_D(\mathbf{x}') d^3x \, d^3x' \tag{2.26}$$

representing the (instantaneous) Coulomb interaction.

When the particle field operators are expanded as in Eq. (2.18), one sees that H_C can be expressed as a "no-pair" interaction plus a remainder. The former may be combined with H_0, giving a new "unperturbed" Hamiltonian whose eigenstates define the no-pair approximation. Corrections are obtained through a modified perturbation expansion accounting for the creation and annihilation of electron-positron pairs as well as the effects of transverse-photon exchange.

B. Effective potential in second order

To provide a simple illustration of the formalism just developed and to establish notation that will be used later on, we now determine the effective potential in second order. To do this we first evaluate the sum of matrix elements

$$\langle n'|H_C|n\rangle + \langle n'|H_T(E-H_0)^{-1}H_T|n\rangle \ .$$

After removal of vacuum components this combination gives the second-order contribution to $F_{n'n}(E)$, Eq. (2.5). The effective potential is then obtained from Eq. (2.17).

We begin with some definitions. The electron propagator is given by

$$s^{(+)}(\mathbf{x},\mathbf{x}';E) = \sum_q^{(+)} \frac{u_q(\mathbf{x}) u_q^\dagger(\mathbf{x}')}{E - \varepsilon_q + i\eta} \ , \tag{2.27}$$

and the positron propagator is

$$s^{(-)}(\mathbf{x},\mathbf{x}';E) = \sum_q^{(-)} \frac{v_q(\mathbf{x}) v_q^\dagger(\mathbf{x}')}{E - |\varepsilon_q| + i\eta} \ , \tag{2.28}$$

with η a positive infinitesimal. The transverse-photon propagator is

$$p_{ii'}(\mathbf{x},\mathbf{x}';E) = \sum_s \frac{1}{2k_s} \frac{U_{si}(\mathbf{x}) \mathbf{U}_{si'}^*(\mathbf{x}')}{E - k_s + i\eta} \ , \tag{2.29}$$

where U_{si} is given by Eq. (2.22) with the polarization vector $\mathbf{e}^{\lambda_s}$ replaced by its ith Cartesian component.

The second-order effective potential $M^{(2)}(\mathbf{x},\mathbf{x}';E)$ is the sum of six terms which are represented diagrammatically in Fig. 1. The Coulomb interaction generates the contri-

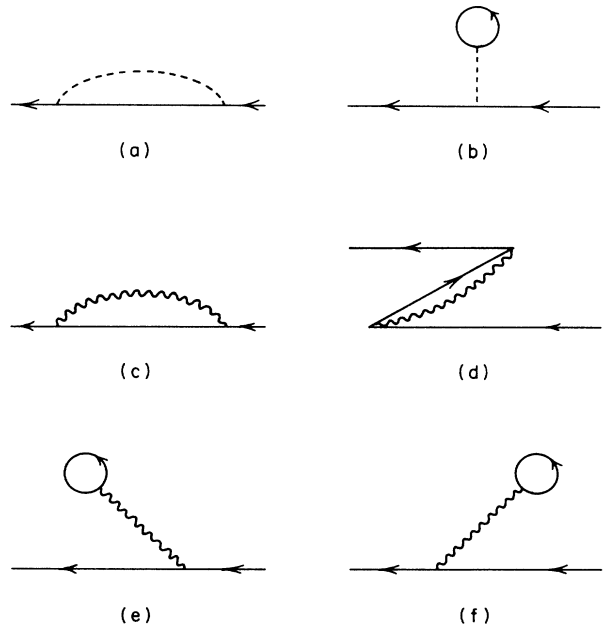

FIG. 1. Diagrammatic representation of the contributions to the effective potential in second order. The Coulomb interaction is represented by a dashed line, transverse-photon propagation by a wavy line, and solid lines represent electron or positron propagation. Diagrams (a), (c), and (d) describe fluctuation effects and diagrams (b), (e), and (f) correspond to the effect of vacuum polarization in the presence of an external field.

bution M_a+M_b with[14]

$$M_a(\mathbf{x},\mathbf{x}';E)=\int L^{(+)}(\mathbf{x},\mathbf{y})L^{(+)}(\mathbf{y},\mathbf{y}')\frac{e^2}{4\pi|\mathbf{y}-\mathbf{y}'|}\times L^{(+)}(\mathbf{y}',\mathbf{x}')d^3y\,d^3y' , \tag{2.30}$$

$$M_b(\mathbf{x},\mathbf{x}';E)=\int L^{(+)}(\mathbf{x},\mathbf{y})[\mathrm{Tr}\bar{L}(\mathbf{y},\mathbf{y}')]\frac{e^2}{4\pi|\mathbf{y}-\mathbf{y}'|}\times L^{(+)}(\mathbf{y}',\mathbf{x}')d^3y\,d^3y' . \tag{2.31}$$

Here $\bar{L}(\mathbf{x},\mathbf{x}')\equiv[L^{(-)}(\mathbf{x},\mathbf{x}')-L^{(+)}(\mathbf{x},\mathbf{x}')]/2$, where

$$L^{(+)}(\mathbf{x},\mathbf{x}')=\sum_n^{(+)} u_n(\mathbf{x})u_n^\dagger(\mathbf{x}') \tag{2.32}$$

is the projection operator onto positive-energy states and

$$L^{(-)}(\mathbf{x},\mathbf{x}')=\sum_m^{(-)} v_m(\mathbf{x})v_m^\dagger(\mathbf{x}') \tag{2.33}$$

is the negative-energy projection operator.[15] The vacuum-fluctuation contribution arising from the emission and reabsorption of a transverse photon is M_c+M_d, with

$$M_c(\mathbf{x},\mathbf{x}';E)=\sum_{i,i'}\int L^{(+)}(\mathbf{x},\mathbf{y})e\alpha_i p_{ii'}(\mathbf{y},\mathbf{y}';E)*s^{(+)}(\mathbf{y},\mathbf{y}';E)\times e\alpha_{i'}L^{(+)}(\mathbf{y}',\mathbf{x}')d^3y\,d^3y' , \tag{2.34}$$

and

$$M_d(\mathbf{x},\mathbf{x}';E)=-\sum_{i,i'}\int s^{(+)}(\mathbf{x},\mathbf{y};E)*e\alpha_i s^{(-)}(\mathbf{y},\mathbf{y}';E)*p_{ii'}(\mathbf{y}',\mathbf{y};E)e\alpha_{i'}*s^{(+)}(\mathbf{y}',\mathbf{x}';E)d^3y\,d^3y' . \tag{2.35}$$

(Note that the convolution operator is associative and commutative.) Finally, the transverse-photon contribution to the vacuum-polarization effect is M_e+M_f, with

$$M_e(\mathbf{x},\mathbf{x}';E)=\sum_{i,i'}\int \mathrm{Tr}[\bar{L}(\mathbf{y}',\mathbf{y}')e\alpha_i]s^{(+)}(\mathbf{x},\mathbf{y};E)*p_{ii'}(\mathbf{y}',\mathbf{y};E)\times e\alpha_{i'}L^{(+)}(\mathbf{y},\mathbf{x}')d^3y\,d^3y' , \tag{2.36}$$

and

$$M_f(\mathbf{x},\mathbf{x}';E)=\sum_{i,i'}\int L^{(+)}(\mathbf{x},\mathbf{y})e\alpha_i p_{ii'}(\mathbf{y},\mathbf{y}';E)*s^{(+)}(\mathbf{y},\mathbf{x}';E)\times \mathrm{Tr}[\bar{L}(\mathbf{y}',\mathbf{y}')e\alpha_{i'}]d^3y\,d^3y' . \tag{2.37}$$

The appearance of the symmetrized projection operator $\bar{L}$ in Eqs. (2.31), (2.36), and (2.37) results from the use of symmetrized charge and current operators (which has the consequence that the vacuum-polarization effect vanishes in the absence of an external field, as it should).[16]

Coulomb and transverse-photon propagators may be combined in the form of a photon propagator identical to that which appears in the covariant formulation in the Coulomb gauge.[17] For example, the fluctuation terms shown in Figs. 1(a) and 1(c) may be combined in the form

$$M_a(\mathbf{x},\mathbf{x}';E)+M_c(\mathbf{x},\mathbf{x}';E)=\sum_{\mu=0}^{3}\sum_{\mu'=0}^{3}\int L^{(+)}(\mathbf{x},\mathbf{y})e\alpha_\mu P_{\mu\mu'}(\mathbf{y},\mathbf{y}';E)\times e\alpha_{\mu'}L^{(+)}(\mathbf{y}',\mathbf{x}')d^3y\,d^3y' . \tag{2.38}$$

Here we introduced the propagator

$$P_{\mu\mu'}(\mathbf{y},\mathbf{y}';E)=p_{\mu\mu'}(\mathbf{y},\mathbf{y}';E)*s^{(+)}(\mathbf{y},\mathbf{y}';E) \tag{2.39}$$

for a photon in the presence of a spectator electron; α_0 is defined as the unit 4×4 matrix, and

$$p_{00}(\mathbf{y},\mathbf{y}';E)=\frac{1}{4\pi|\mathbf{y}-\mathbf{y}'|} , \tag{2.40}$$

with $p_{0i}=p_{i0}=0$, $i=1,2,3$. The wavy line in Fig. 1(c) representing the transverse-photon propagator will, in diagrams introduced later on, be understood to represent the combined Coulomb-transverse-photon propagator.

The level shift in second order is obtained from the expectation value of $M^{(2)}(\mathbf{x},\mathbf{x}';\varepsilon_n)$ in the state $|n\rangle$. An exact correspondence with the covariant expression for this level shift[18] may be established by inserting the Fourier transforms of the photon and electron propagators which appear in the latter expression (these transforms are given in the Appendix) and then carrying out the integrations over the time and energy variables. This correspondence allows one to set up a renormalization prescription for the second-order level shift in the Hamiltonian formulation parallel to the Coulomb-gauge version of the covariant prescription.[10] Use of the Hamiltonian formalism is likely to provide computational advantages in the calculation of higher-order corrections, particularly in the evaluation of sums over low-energy intermediate states[19] in which the instantaneous Coulomb interaction plays the dominant role. In the following, we attempt to put this observation in more specific form through an analysis of the one-pair approximation.

One must recognize, of course, the danger in too strict an enforcement of the limitation to intermediate states of a particular type. Thus in a no-pair approximation the contribution to the effective potential shown in Fig. 1(d) would be omitted with a resultant loss of covariance and renormalizability of the self-energy. Similarly, in a one-pair approximation the fourth-order diagrams of Figs. 2(a) and 2(b) are included but those shown in Figs. 2(c) and 2(d), which differ only in the "time"-ordering, would be omitted since they contain two-photon intermediate states; this would leave nonrenormalizable self-energy functions. In the following, the one-pair model is adopted in a strict form—only intermediate states consisting

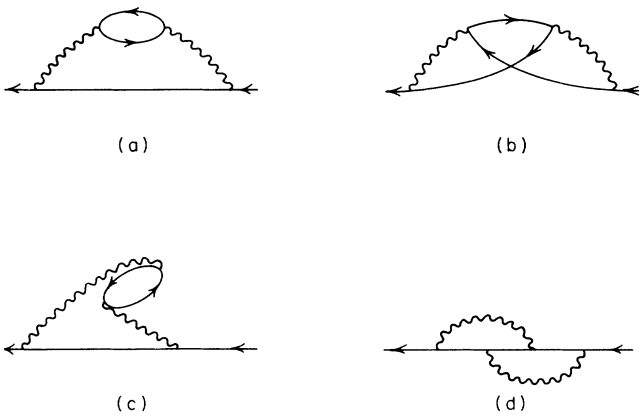

FIG. 2. Fourth-order terms represented by diagrams (a) and (b) contribute to the effective potential in the one-pair model. Diagrams (c) and (d) represent terms which arise from different time orderings; they contain two-photon intermediate states and are omitted in the one-pair model as defined in Sec. III of the text. (Wavy lines in this figure stand for the combined Coulomb-transverse-photon propagator.)

of an electron plus a pair, or an electron plus a photon, will be introduced. This is done to simplify and focus the discussion; it will be understood implicitly that the model must eventually be enlarged to include all time-orderings necessary for renormalizability.

III. ONE-PAIR APPROXIMATION

A. Description of the model

The effective potential in the one-pair model is defined by an infinite collection of perturbation terms corresponding to a restricted class of intermediate states. These terms may be formally summed using integral equations which, upon iterative solution, generate the desired series expansion. The effect of repeated pair interactions is accounted for through the introduction of two-body Green's functions. Successive interactions involving different pairs are summed with the aid of three-body integral equations of the Faddeev-Watson type.[20] These integral equations could be used as the basis for numerical computation. Here, however, they are introduced merely as a technical device which facilitates the separation of one-photon intermediate-state contributions to the electron-positron Green's function from the (nondivergent) remainder. This leads to the definition of an irreducible kernel, the K matrix, which describes the Coulomb interaction of the three-body system and which can be calculated by means of a Rayleigh-Ritz variational procedure. The details of this analysis will not be presented here. (A very similar derivation was used previously in the development of an effective-potential formulation of the nonrelativistic three-body scattering problem.[21]) Rather, in this section we write down the final form of the integral equations and define the various components (kernels, propagators, vertex functions) in terms of which these equations are expressed. The minimum principle for the K matrix is derived in Sec. III B.

Fourth-order contributions to the one-electron effective potential $M(\mathbf{x},\mathbf{x}';E)$ in the one-pair approximation are pictured in Figs. 2(a) and 2(b). (Self-energy corrections to internal electron lines, omitted here, must ultimately be included self-consistently.) The pair-annihilation vertex appearing in these diagrams has associated with it the (lowest-order) vertex function

$$\tilde{\xi}_\mu(\mathbf{x};\mathbf{y},\mathbf{z})=L^{(-)}(\mathbf{z},\mathbf{x})e\alpha_\mu L^{(+)}(\mathbf{x},\mathbf{y}) , \tag{3.1}$$

and the pair-creation vertex is represented by

$$\xi_\mu(\mathbf{y},\mathbf{z};\mathbf{x})=L^{(+)}(\mathbf{y},\mathbf{x})e\alpha_\mu L^{(-)}(\mathbf{x},\mathbf{z}) . \tag{3.2}$$

Figure 2(a) shows a self-energy correction to the photon propagator. This, together with higher-order iterations in the one-pair model, gives rise to the vacuum fluctuation diagram of Fig. 3(a); the modified photon propagator is given by the sum of "bubble" diagrams shown in Fig. 3(b). With the photon self-energy denoted as $\pi_{\mu\nu}(\mathbf{x},\mathbf{x}';E)$—it is defined explicitly in Sec. III B—the sum may be represented as the solution of the integral equation

$$p'_{\mu\mu'}(\mathbf{x},\mathbf{x}';E)=p_{\mu\mu'}(\mathbf{x},\mathbf{x}';E)+\sum_{\nu,\nu'}\int p_{\mu\nu}(\mathbf{x},\mathbf{y};E)\pi_{\nu\nu'}(\mathbf{y},\mathbf{y}';E)\times p'_{\nu'\mu'}(\mathbf{y}',\mathbf{x}';E)d^3y\,d^3y' . \tag{3.3}$$

The one-electron effective potential in the one-pair model is of the form

$$M_{1p}(\mathbf{x},\mathbf{x}';E)\equiv\int L^{(+)}(\mathbf{x},\mathbf{y})\Sigma(\mathbf{y},\mathbf{y}';E)\times L^{(+)}(\mathbf{y}',\mathbf{x}';E)d^3y\,d^3y' . \tag{3.4}$$

The contribution to Σ corresponding to the fluctuation diagram of Fig. 3(a) is

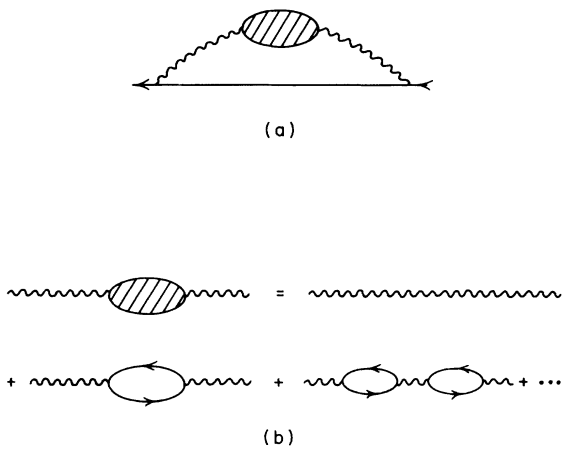

FIG. 3. Diagram (a) represents a vacuum-fluctuation contribution to the one-electron effective potential. The modified photon propagator appearing there is pictured as the sum of "bubble" diagrams in diagram (b).

$$\Sigma_F(\mathbf{x},\mathbf{x}';E)=\int \tilde{\Gamma}_\mu^{(0)}(\mathbf{x};\mathbf{y},\mathbf{z})P'_{\mu\nu}(\mathbf{y},\mathbf{z};\mathbf{y}',\mathbf{z}';E)\Gamma_\nu^{(0)}(\mathbf{y}',\mathbf{z}';\mathbf{x}') . \tag{3.5}$$

(To simplify notation, here and in the following a single integration sign will imply the instruction to carry out the sums over repeated photon indices and integration over repeated position labels.) In Eq. (3.5) we have introduced the electron-photon propagator

$$P'_{\mu\nu}(\mathbf{y},\mathbf{z};\mathbf{y}',\mathbf{z}';E)=p'_{\mu\nu}(\mathbf{y},\mathbf{y}';E)*s^{(+)}(\mathbf{z},\mathbf{z}';E) , \tag{3.6}$$

along with the bare vertex functions

$$\tilde{\Gamma}_\mu^{(0)}(\mathbf{x};\mathbf{y},\mathbf{z})=\Gamma_\mu^{(0)}(\mathbf{y},\mathbf{z};\mathbf{x})\equiv e\alpha_\mu\delta(\mathbf{x}-\mathbf{y})\delta(\mathbf{x}-\mathbf{z}) . \tag{3.7}$$

The lowest-order contribution to the remainder $\Sigma-\Sigma_F$ is the term pictured in Fig. 2(b). To this we add the contribution obtained by including all Coulomb interactions in intermediate states of the $e^-e^-e^+$ system. In addition, we must account for the fact that the positron can interact with each of the electrons through the annihilation and creation mechanism and its iterations. It is important to isolate these divergent photon self-energy parts. This is accomplished by expressing the kernel Σ in the form

$$\Sigma(\mathbf{x},\mathbf{x}';E)=\int \tilde{\Gamma}_\mu^{(0)}(\mathbf{x};\mathbf{y},\mathbf{z})P'_{\mu\nu}(\mathbf{y},\mathbf{z};\mathbf{y}',\mathbf{z}';E)\Gamma_\nu(\mathbf{y}',\mathbf{z}';\mathbf{x};E) . \tag{3.8}$$

Here Γ_μ is a modified vertex function satisfying the integral equation

$$\Gamma_\mu(\mathbf{y},\mathbf{z};\mathbf{x};E)=\Gamma_\mu^{(0)}(\mathbf{y},\mathbf{z};\mathbf{x}) + \int K_{\mu\nu}(\mathbf{y},\mathbf{z};\mathbf{y}',\mathbf{z}';E)P'_{\nu\nu'}(\mathbf{y}',\mathbf{z}';\mathbf{y}'',\mathbf{z}'';E) \times\Gamma_{\nu'}(\mathbf{y}'',\mathbf{z}'';\mathbf{x};E) . \tag{3.9}$$

The kernel K sums all photon-electron interactions evolving through intermediate states consisting only of an electron and a pair. Photon-electron intermediate states appear only in the propagator P' in Eqs. (3.8) and (3.9); they are excluded from the K matrix. For later reference we note that an alternative version of Eq. (3.8) is (with position labels now completely suppressed, and sums over repeated indices implied)

$$\Sigma(E)=\tilde{\Gamma}_\mu(E)P'_{\mu\nu}(E)\Gamma_\nu^{(0)}(E) , \tag{3.10}$$

where $\tilde{\Gamma}_\mu$ satisfies the adjoint version of Eq. (3.9).

An explicit expression for the kernel K is obtained in the course of the analysis leading to Eqs. (3.8) and (3.9). To write it down we need some additional notation. We are dealing with a system of two electrons (particles 1 and 2) and a positron (particle 3) interacting through pairwise Coulomb potentials in the presence of an external (nuclear) potential. The appropriate Hamiltonian is

$$H_C=h(1)+h(2)-h(3)+V_C . \tag{3.11}$$

Here $h(i)$ is the Dirac Hamiltonian, Eq. (2.11b), for the ith particle and $V_C=v_1+v_2+v_3$, with v_1 representing the Coulomb interaction between particles 2 and 3, etc. If only the ith pair is interacting, the relevant Hamiltonian is $H_{Ci}=h(1)+h(2)-h(3)+v_i$. These operators act in a subspace projected onto by the operator $L^{(+)}(1)L^{(+)}(2)L^{(-)}(3)$. The associated Green's functions are

$$G(E)=(E-H_C)^{-1} , \tag{3.12}$$

and

$$G_i(E)=(E-H_{Ci})^{-1} . \tag{3.13}$$

Note that $G_1(E)$, for example, is the convolution

$$G_1(E)=g_1(E)*s^{(+)}(1;E) , \tag{3.14}$$

where $s^{(+)}(1;E)$ is the propagator for the spectator electron and $g_1(E)$ is the Coulomb Green's function of electron 2 and the positron. We now introduce, for $i=1$ or 2, the function

$$\phi_{\mu i}(\mathbf{y}',\mathbf{z}';\mathbf{x};E)=\int g_i(\mathbf{y}',\mathbf{z}';\mathbf{y},\mathbf{z};E)\xi_{\mu i}(\mathbf{y},\mathbf{z};\mathbf{x}) , \tag{3.15}$$

and its adjoint

$$\tilde{\phi}_{\mu i}(\mathbf{x};\mathbf{y}',\mathbf{z}';E)=\int \tilde{\xi}_{\mu i}(\mathbf{x};\mathbf{y},\mathbf{z})g_i(\mathbf{y},\mathbf{z};\mathbf{y}',\mathbf{z}';E) ; \tag{3.16}$$

$\tilde{\xi}_{\mu i}$ and $\xi_{\mu i}$ are the vertex functions defined in Eqs. (3.1) and (3.2). To study the structure of Eq. (3.15) in more detail we write, in condensed notation, with pair index omitted, $\phi_\mu=g\xi_\mu$ and observe that g satisfies the linear integral equation $g=g_0+g_0vg$; g_0 is the free Green's function for the pair. An iterative solution for g leads to the expansion $\phi_\mu=g_0(\xi_\mu+vg_0\xi_\mu+\cdots)$. In going beyond the leading term divergence difficulties arise which must be treated by renormalization procedures. To do this properly one must include vertex corrections arising from transverse-photon exchange in addition to the Coulomb corrections indicated explicitly above. Renormalization can then proceed along standard lines; use of the Coulomb gauge introduces no obstacles.[10] Without pursuing the matter further here we emphasize that with the divergent vertex function and photon self-energy function isolated, we are left with a well-defined calculational problem—construction of the K matrix—which we now consider.

The electrons may be treated, temporarily, as distinguishable particles with the properly antisymmetrized K matrix then formed as the difference between direct and exchange amplitudes. Thus the K matrix appearing in Eq. (3.9) is given by

$$K_{\mu\mu'}=K^{11}_{\mu\mu'}-K^{21}_{\mu\mu'} , \tag{3.17}$$

where $K^{ij}_{\mu\mu'}, i,j=1,2$, corresponds to an electron-photon interaction in which electron j and a photon of index μ' appears in the initial state, and electron i along with a photon of index μ emerge in the final state. Here we use the language of scattering theory, and if we continue to do so we may say that the initial-state "wave function" is

$$\Phi_{\mu' j}(E)=\phi_{\mu' j}(E)*s^{(+)}(j;E) \tag{3.18}$$

and the final-state wave function is

$$\tilde{\Phi}_{\mu i}(E)=\tilde{\phi}_{\mu i}(E)*s^{(+)}(i;E) \tag{3.19}$$

(with ϕ and $\bar{\phi}$ playing the role of target bound-state wave functions). We find from our analysis of the one-pair model that the K matrix is given by

$$K^{ij}_{\mu\mu'}(E)=\tilde{\Phi}_{\mu i}(E)\left[(E-H_C+V_C)(1-\delta_{ij})+\sum_{m\neq i,j}v_m+(V_C-v_i)G(E)(V_C-v_j)\right]\Phi_{\mu' j}(E)\ , \tag{3.20}$$

where position variables have been suppressed to simplify the writing.

B. Variational principles and minimum principles

The Green's functions $g_i(E)$ and $G(E)$ which appear in Eqs. (3.15) and (3.20) each satisfy a minimum principle and this can be useful in the approximate evaluation of matrix elements in which these functions appear. The photon self-energy, for example, has the form

$$\pi_{\mu\mu'}(\mathbf{x},\mathbf{x}';E)=\int\bar{\xi}_{\mu}(\mathbf{x};\mathbf{y},\mathbf{z})g(\mathbf{y},\mathbf{z};\mathbf{y}',\mathbf{z}';E)\xi_{\mu'}(\mathbf{y}',\mathbf{z}';\mathbf{x}') \tag{3.21}$$

in the one-pair model. A minimum principle for g can (after suitable regularization of the integrals) be translated into a minimum principle for diagonal elements of the self-energy matrix; the trial functions determined in the course of the calculation provide approximate solutions of Eqs. (3.15) and (3.16). The utility of the minimum principle lies in the fact that it provides a criterion for the optimum choice of variational parameters which appear in the trial functions. Similar remarks can be made with regard to the construction of the K matrix defined in Eq. (3.20).

To develop this point in more detail we observe that the Green's function in Eq. (3.20) satisfies the identity

$$G(E)=G_t(E)+G(E)[1+(H_C-E)G_t(E)]\ , \tag{3.22}$$

with $G_t(E)$ representing a trial estimate of $G(E)$. With G on the right-hand side of Eq. (3.22) replaced by $G_t+\Delta G$, the identity becomes

$$G=G_v-\Delta G(H_C-E)\Delta G\ , \tag{3.23}$$

where

$$G_v=G_t+G_t[1+(H_C-E)G_t]\ . \tag{3.24}$$

With ΔG assumed to be a quantity of first order, the error $G-G_v$ is of second order so that G_v represents a variational estimate of G. Moreover, since E lies well below the minimum eigenvalue of H_C,[22] the error is a negative operator. That is, diagonal matrix elements of the error will be negative, and this provides the basis for the minimum principle. Let us define the trial functions

$$\Psi_{\mu' j}=G_t(V_C-v_j)\Phi_{\mu' j} \tag{3.25}$$

and

$$\tilde{\Psi}_{\mu i}=\tilde{\Phi}_{\mu i}(V_C-v_i)G_t\ . \tag{3.26}$$

With G replaced by its variational estimate in Eq. (3.20), we obtain a variational approximation for the K matrix of the form

$$K^{ij}_{\mu\mu'}=\tilde{\Phi}_{\mu i}\left[(E-H_C+V_C)(1-\delta_{ij})+\sum_{m\neq i,j}v_m\right]\Phi_{\mu' j}+\tilde{\Phi}_{\mu i}(V_C-v_i)\Psi_{\mu' j}+\tilde{\Psi}_{\mu i}(V-v_j)\Phi_{\mu' j}+\tilde{\Psi}_{\mu i}(H_C-E)\Psi_{\mu' j}\ . \tag{3.27}$$

The error is

$$\Delta K^{ij}_{\mu\mu'}=-\Delta\tilde{\Psi}_{\mu i}(H_C-E)\Delta\Psi_{\mu' j}\ . \tag{3.28}$$

This is not diagonal in the particle indices i and j, but the antisymmetrized combination shown in Eq. (3.17) can in fact be represented as the diagonal matrix element

$$K_{\mu\mu'}=\underline{a}^{\dagger}\underline{K}_{\mu\mu'}\underline{a}\ , \tag{3.29}$$

where $\underline{K}_{\mu\mu'}$ is the 2×2 matrix with elements $K^{ij}_{\mu\mu'}$ and

$$\underline{a}=\frac{1}{\sqrt{2}}\begin{bmatrix}1\\-1\end{bmatrix}\ . \tag{3.30}$$

The minimum principle applies to $K_{\mu\mu}(\mathbf{y},\mathbf{z};\mathbf{y},\mathbf{z};E)$.

The result just obtained is not yet in its most useful form since the minimum principle applies only to elements which are diagonal, in position variables as well as photon indices. A more satisfactory (though necessarily more elaborate) procedure is one which relates K directly to the energy eigenvalue—the number of physical interest—and which preserves the minimum principle. As a first step toward a formulation of this procedure we invoke the Rayleigh-Ritz principle for determining the energy eigenvalue from the modified one-electron Dirac equation, Eq. (2.16). With the energy parameter in the effective potential M fixed at a trial value $\hat{E}_{nt}$, we have the estimate

$$\hat{E}_{nv}=\int\psi^{\dagger}_{nt}(\mathbf{x})[h(\mathbf{x})\delta(\mathbf{x}-\mathbf{x}')+M(\mathbf{x},\mathbf{x}';\hat{E}_{nt})]\psi_{nt}(\mathbf{x}')\ , \tag{3.31}$$

where ψ_{nt} is a normalized trial solution of Eq. (2.16) satisfying $L^{(+)}\psi_{nt}=\psi_{nt}$. Suppose that a trial function ψ_{nt} has been chosen, based on some first (perhaps crude) estimate of the kernel M, and we wish to improve on the calculation through a more refined determination of M. Actually, we may focus our attention on Σ since $M-\Sigma$ is just a sum of second-order terms [shown in diagrams (b) and (d)–(f) of Fig. 1] which may be assumed to be known. We consider, therefore, the problem of estimating the diagonal matrix element $\psi^{\dagger}_{nt}\Sigma(\hat{E}_{nt})\psi_{nt}$ for a given ψ_{nt}. (Here we revert to the condensed notation in which integration variables are suppressed.) The kernel Σ is defined in Eq. (3.8). A variational principle for Σ (the dependence on the energy parameter $\hat{E}_{nt}$ will be left implicit) is provided by the expression

$$\Sigma_v=\tilde{\Gamma}^{(0)}_{\mu}P'_{\mu\nu}\Gamma_{\nu t}+\tilde{\Gamma}_{\mu t}P'_{\mu\nu}\Gamma^{(0)}_{\nu}+\tilde{\Gamma}_{\mu t}(P'_{\mu\sigma}K_{\sigma\rho}P'_{\rho\nu}-P'_{\mu\nu})\Gamma_{\nu t}\ , \tag{3.32}$$

which is stationary about the exact expression (3.8) under independent variations of $\Gamma_{\mu t}$ about the exact solution of Eq. (3.9) and of $\tilde{\Gamma}_{\mu t}$ about the exact solution of the adjoint of Eq. (3.9). [In verifying that first-order variations of Σ_v vanish, one makes use of Eqs. (3.8) and (3.10) for

Σ.] Of course, the exact K matrix is unknown, and must be determined by an iterative procedure, which might proceed along the following lines. Let $K^{(1)}$ be a first estimate, obtained, for example, from the variational expression (3.27). Trial functions $\Gamma_{\mu t}$ and $\tilde{\Gamma}_{\mu t}$ are constructed variationally from Eq. (3.32) with $K^{(1)}$ as input. An improved estimate $K^{(2)}$ is generated by substitution of the variational expression (3.27) for K into Eq. (3.32). The optimum choice of parameters appearing in the trial functions $\tilde{\Psi}_{\mu i}$ and $\Psi_{\mu' j}$ in Eq. (3.27) are found by minimizing the diagonal matrix element

$$\psi_{nt}^{\dagger}\tilde{\Gamma}_{\mu t}P'_{\mu\sigma}K^{(2)}_{\sigma\rho}P'_{\rho\nu}\Gamma_{\nu t}\psi_{nt} \ .$$

If necessary, the process may be repeated with $K^{(2)}$ as the initial choice. Thus the minimum principle for the K matrix may be imbedded in a well-defined variational scheme leading to the evaluation of the ground-state energy eigenvalue in the one-pair model. The procedure may be modified in a straightforward manner to allow for the determination of excited-state energy levels.

IV. SUMMARY

An analysis has been presented of the one-pair model for a hydrogenic atom based on a time-independent Hamiltonian formulation of QED. The effective one-electron potential has been defined for this model and the integral equations required for its construction have been derived—they provide an analog of the Dyson-Schwinger equations of covariant QED. An advantage of this integral-equation approach lies in the fact that it allows for a separation of the various divergent quantities which appear as elements of the calculation from those which are finite. With this separation accomplished it becomes possible to set up a rigorous Rayleigh-Ritz principle for the evaluation of that nondivergent quantity, referred to here as the K matrix, which plays a central role in the theory. The K matrix contains the effects of the instantaneous Coulomb interactions in a system consisting of two electrons and a positron in the presence of the fixed nuclear charge.

In assessing the potential utility of the time-independent Hamiltonian approach one must first acknowledge that the divergence difficulties have yet to be fully resolved. For one thing, the isolation of multiparticle Coulomb interactions in the construction of the K matrix is not a covariant procedure. These Coulomb interactions, however, are very likely to be significant for only a restricted range of energies of the particles which appear in intermediate states. At very high energies covariant treatments, in which the dynamical complexity of the Coulomb interaction is omitted, may suffice and these allow for renormalization by standard methods. (Ideas along similar lines, involving a separation of covariant and noncovariant contributions, were successfully implemented in previous studies of the Lamb shift in hydrogen[23,18] and helium.[24,25]) An attempt to resolve the divergence problem would seem to be well worthwhile since the Hamiltonian method appears to be computationally simpler than strictly covariant treatments based, for example, on generalized Bethe-Salpeter equations. It provides, furthermore, a natural extension of the Fock-Dirac techniques currently in use, allowing for a study of the range of validity of these techniques and for the introduction of corrections when greater accuracy is required.

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APPENDIX

We specify here the relations between the time-independent noncovariant propagators used in the text and the standard covariant forms. (We use the notation of Jauch and Rohrlich,[11] for the latter.) Let $S_c(x,x')$ represent the causal electron propagator which includes the effect of the external potential $V_{\rm ext}(\mathbf{x})$. The time-evolution operator for the electron is then given by $U_c(\mathbf{x},\mathbf{x}';t-t')=S_c(x,x')\beta$. The Fourier transform is

$$U_c(\mathbf{x},\mathbf{x}';t-t)=-\frac{1}{2\pi i}\int_{-\infty}^{\infty}dE\, s(\mathbf{x},\mathbf{x}';E)e^{-iE(t-t')} \ , \tag{A1}$$

with

$$s(\mathbf{x},\mathbf{x}';E)=\sum_q^{(+)}\frac{u_q(\mathbf{x})u_q^{\dagger}(\mathbf{x}')}{E-\varepsilon_q+i\eta}+\sum_q^{(-)}\frac{v_q(\mathbf{x})v_q^{\dagger}(\mathbf{x}')}{E-\varepsilon_q-i\eta} \ . \tag{A2}$$

The projection operators defined in Eqs. (2.32) and (2.33) are given by

$$L^{(\pm)}(\mathbf{x},\mathbf{x}')=\pm\lim_{\eta\to 0+}U_c(\mathbf{x},\mathbf{x}';\eta) \ .$$

The causal photon propagator is represented as

$$D_{\mu\nu}(x-x')=(2\pi)^{-4}\int D_{\mu\nu}(k)e^{ik(x-x')}d^4k \ . \tag{A3}$$

In the Coulomb gauge we have

$$\begin{aligned} &D_{00}(k)=|\mathbf{k}|^{-2} \ , \\ &D_{ii'}(k)=(-k^2+i\eta)^{-1}\sum_{\lambda}e_i^{\lambda}e_{i'}^{\lambda} \ , \end{aligned} \tag{A4}$$

and $D_{i0}=D_{0i}=0$. From this we obtain

$$\begin{aligned} &D_{00}(x-x')=\frac{1}{4\pi|\mathbf{x}-\mathbf{x}'|}\delta(x_0-x_0') \ , \\ &D_{ii'}(x-x')=\frac{1}{2\pi}\int_{-\infty}^{\infty}dE\, d_{ii'}(\mathbf{x},\mathbf{x}';E)e^{-iE(t-t')} \ ; \end{aligned} \tag{A5}$$

reverting to box normalization for the radiative field we have

$$d_{ii'}(\mathbf{x},\mathbf{x}';E)=\sum_s\frac{U_{si}(\mathbf{x})U_{si'}^{*}(\mathbf{x}')}{E^2-|\mathbf{k}_s|^2+i\eta} \ , \tag{A6}$$

with $\mathbf{U}_s(\mathbf{x})$ given in Eq. (2.22). With the substitution

$$\begin{aligned} &(E^2-|\mathbf{k}_s|^2+i\eta)^{-1} \\ &\quad=(2|\mathbf{k}_s|)^{-1}[(E-|\mathbf{k}_s|+i\eta)^{-1}-(E+|\mathbf{k}_s|-i\eta)^{-1}] \ , \end{aligned} \tag{A7}$$

the expression (A6) for $d_{ii'}$ becomes the sum of two terms, corresponding to photon propagation forward in time [that is just the term $p_{ii'}$ given in Eq. (2.29)] and propagation backward in time, in analogy with the decomposition shown in Eq. (A2) for the electron propagator. These decompositions are useful in the evaluation of the covariant second-order vacuum-fluctuation contribution to the electron self-energy. Integration over the time and energy variables is easily carried out with the aid of the representations of the electron and photon propagators given above. The result is just the sum of M_c and M_d, the noncovariant amplitudes defined in Eqs. (2.34) and (2.35) and pictured in Figs. 1(c) and 1(d). The correspondence between covariant and noncovariant expressions for the remaining contributions to the second-order self-energy is also established without difficulty.

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[14]Here and in the following it will be understood that divergent integrals are to be regularized (through the introduction, for example, of appropriate cutoffs). A successful renormalization procedure is one which provides physically consistent results independent of all cutoff parameters.

[15]It is possible to formulate the problem in terms of projection operators onto the positive- and negative-energy solutions of the *free* Dirac equation (as discussed in Refs. 2 and 6). Since these are simpler to evaluate than the $L^{(\pm)}$ operators, such a formulation may be preferable in practice. We work here with $L^{(+)}$ and $L^{(-)}$ since pair creation by the external potential is then implicitly accounted for to all orders, and this simplifies the presentation of the theory.

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