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Quantum fluctuations and the variational approach to bound states

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Relativistic Hartree-Fock equations are proposed which incorporate radiative effects. Their derivation is based on functional integration methods and a new substitution rule inferred from the Pauli principle.

I. INTRODUCTION

Variational approximations play a central role in the treatment of bound states in quantum field theory. Motivated by the hope of arriving at a description of hadrons as bound states of quarks in the framework of field theory, new variational approaches have been investigated during recent years.[1-3] Various techniques have been employed based either on conventional Fock-space methods or on the Feynman path-integral representation of the generating functional. Using functional integration methods, Dashen *et al.*[2] derived self-consistent-field (SCF) equations in a two-dimensional model field theory. These equations describe effects from vacuum polarization, thus including quantum fluctuations in a variational procedure.

The incorporation of radiative corrections in relativistic SCF equations is one of the main theoretical problems in atomic physics.[4] Radiative corrections are tested by several types of experiments involving strong external fields,[5] heavy atoms[6] or heliumlike ions.[7] In contrast to the one-electron problem (hydrogenlike ions), which has been treated rigorously on the basis of quantum electrodynamics (QED),[8,9] a systematic treatment of many-electron bound states in the framework of QED does not exist.[10] It is not known even in principle how energy spectra can be calculated for bound states of more than one constituent in a systematic perturbation theory including relativistic and radiative effects. At present the incorporation of radiative effects in variational approximations of Hartree-Fock type seems the best one can do. This approach has been discussed in the literature,[5,11-15] in particular by Reinhard, Greiner, and Arenhövel[13] and Rafelski, Müller, and Greiner.[14] In this paper the new variational methods mentioned above are applied to the many-electron bound-state problem in QED. The results are similar to those obtained in Ref. 14. There are, however, differences as far as the treatment of quantum fluctuations is concerned. Rafelski *et al.* treat "sea" electrons self-consistently, in the same way as bound electrons; this leads to an infinite number of coupled integro-differential equations. The approach presented in this paper yields SCF equations for the bound constituents only, whereas the "sea" is solely determined by the external potential.

The method developed by Dashen *et al.* to treat bound fermions turns out not to be appropriate for the description of bound states in quantum electrodynamics. The SCF equations obtained by these authors lead to a classical self-interaction of bound constituents which is not observed experimentally. This is very similar to the self-interaction problem encountered in Fock-space variational approximations based on coherent trial states.[16] In both cases self-interaction terms occur because exchange interactions are not taken into account. In this paper a method is presented which yields relativistic Hartree-Fock equations incorporating exchange interactions as well as the effects from quantum fluctuations. This is achieved by using some of the ideas of Dashen *et al.* and a new substitution rule inferred from the Pauli principle.

The main steps of the proposed method are the following: the starting point is the energy $E_{\text{vac}}[A^{\text{ex}}]$ of the vacuum in an external static potential $A_\mu^{\text{ex}}(\vec{x})$, which will be calculated in the one-loop approximation using functional integration techniques in Sec. II. I then derive the substitution rule from the Pauli principle and apply it to the vacuum energy $E_{\text{vac}}[A^{\text{ex}}]$. The result is the energy $E[A^{\text{ex}}; U_1, U_2]$ of a two-electron state in the presence of the external potential A_μ^{ex} in the SCF approximation. Variation of the functional $E[A^{\text{ex}}; U_1, U_2]$ with respect to the "wave functions" U_1, U_2 of the bound electrons leads to SCF equations determining U_1 and U_2 (Sec. III). A straightforward generalization of the substitution rule employed for the two-electron system yields Hartree-Fock equations for an arbitrary number of bound electrons and positrons (Sec. IV). Section V describes how the energy spectrum of bound states can be calculated on the basis of the derived equations. In addition the relation to the work of

Rafelski *et al.*[14] is discussed. I conclude with a summary of my results in Sec. VI. Appendices A and B deal with the method of Dashen *et al.*

II. VACUUM ENERGY IN AN EXTERNAL POTENTIAL

Our starting point is the functional integral

$$W(T)=\frac{1}{N}\int [DA_\mu][D\psi][D\bar{\psi}]\exp(iS[A,\psi,\bar{\psi}])\,, \qquad (2.1)$$

where $S[A,\psi,\bar{\psi}]$ is the action of quantum electrodynamics in a static external potential A_μ^{ex} in the Feynman gauge[17]

$$S[A,\psi,\bar{\psi}]=\int_{t_1}^{t_2} dt\int d^3x\{-\tfrac{1}{2}\partial_\mu A_\nu\partial^\mu A^\nu + \bar{\psi}[\gamma^\mu(i\partial_\mu-eA_\mu^{\mathrm{ex}}-eA_\mu)-m]\psi\}\,; \qquad (2.2)$$

$T=t_2-t_1$, N is a normalization factor, and the integration is restricted to periodic field configurations, i.e.,

$$A_\mu(t_1,\vec{x})=A_\mu(t_2,\vec{x}),\quad \psi(t_1,\vec{x})=\psi(t_2,\vec{x})\,. \qquad (2.3)$$

As the action is bilinear in ψ and $\bar{\psi}$, the integration over the spinor field can be performed immediately, thus incorporating quantum fluctuations of the matter field from the beginning.[18] An integral over the vector field A_μ remains, involving an effective action $S_{\mathrm{eff}}[A]$:

$$W(T)=\frac{1}{N}\int [DA_\mu]\exp(iS_{\mathrm{eff}}[A])\,, \qquad (2.4)$$

where

$$S_{\mathrm{eff}}[A] =\int_{t_1}^{t_2} dt\int d^3x(-\tfrac{1}{2}\partial_\mu A_\nu\partial^\mu A^\nu)-i\,\mathrm{tr}\ln[-i(\not{D}-m)]$$

and

$$\mathrm{Tr}\ln[-i(\not{D}-m)]=\ln\mathrm{Det}[-i(\not{D}-m)]$$

is the logarithm of the determinant of the differential operator

$$-i(\not{D}-m)=-i[\gamma^\mu(i\partial_\mu-eA_\mu^{\mathrm{ex}}-eA_\mu)-m]\,.$$

The calculation of the vacuum energy $E_{\mathrm{vac}}[A^{\mathrm{ex}}]$ now proceeds in the following way: I first demonstrate that the effective action has a time-independent stationary point a_μ corresponding to the vacuum polarization correction to the external potential A_μ^{ex}; I then calculate the contribution of this stationary point to the functional integral $W(T)$ in the one-loop approximation for large values of T; the final step is to identify the vacuum energy as[2,19]

$$E_{\mathrm{vac}}[A^{\mathrm{ex}}]=i\lim_{T\to\infty}\frac{1}{T}\ln W(T)\,. \qquad (2.5)$$

The variational derivative of the effective action reads

$$\frac{\delta}{\delta A_\mu(x)}S_{\mathrm{eff}}[A] =\Box A^\mu(x)+ie\,\mathrm{tr}[\gamma^\mu S(x,x|A^{\mathrm{ex}}+A)]\,, \qquad (2.6)$$

where "tr" denotes the trace with respect to the spinor indices, and the propagator $S(x,y|A)$ is defined by

$$[\gamma^\mu(i\partial_\mu-eA_\mu)-m]S(x,y|A)=\delta^4(x-y)\,. \qquad (2.7)$$

The condition for a stationary point of the effective action,

$$\frac{\delta}{\delta A_\mu(x)}S_{\mathrm{eff}}[A]=0\,,$$

determines a potential $a_\mu(x)$ which, according to Eq. (2.6), is generated by the vacuum polarization current induced by the "classical" potential[20] A_μ^{cl}:

$$\Box a_\mu(x)=-ie\,\mathrm{tr}[\gamma_\mu S(x,x|A^{\mathrm{cl}})]\,,\quad A_\mu^{\mathrm{cl}}=A_\mu^{\mathrm{ex}}+a_\mu\,. \qquad (2.8)$$

For a static external potential A_μ^{ex} the induced vacuum polarization correction a_μ is time independent as well.

To compute $W(T)$ in the one-loop approximation, we expand the effective action around the stationary point $a_\mu(x)$ and neglect terms higher than quadratic in η:

$$S_{\mathrm{eff}}[A]=S_{\mathrm{eff}}[a]+\frac{1}{2!}\int d^4x\,d^4x'\,\eta_\nu(x')\times\frac{\delta^2 S_{\mathrm{eff}}}{\delta A_\nu(x')\delta A_\mu(x)}[a]\eta_\mu(x)+\cdots\,, \qquad (2.9)$$

$$A_\mu=a_\mu+\eta_\mu\,.$$

From Eqs. (2.1), (2.4), and (2.9) we thus obtain[18]

$$W(T)=\frac{1}{N}\exp\left[iS_{\mathrm{eff}}[a] -\tfrac{1}{2}\,\mathrm{tr}\ln\left(-i\frac{\delta^2 S_{\mathrm{eff}}}{\delta A_\nu(x)\delta A_\mu(x')}[a]\right)+\cdots\right], \qquad (2.10)$$

i.e., the determination of $W(T)$ requires the evaluation of the effective action at the stationary point and the computation of a trace involving the second functional derivative of $S_{\mathrm{eff}}[A]$.

Let us start with the trace. Using the relation

$$\frac{\delta}{\delta A_\mu(z)}S(x,y|A)=eS(x,z|A)\gamma^\mu S(z,y|A)\,, \qquad (2.11)$$

we obtain

$$\frac{\delta^2 S_{\mathrm{eff}}}{\delta A_\nu(x')\delta A_\mu(x)} =\Box g^{\mu\nu}\delta^4(x-x')+ie^2\,\mathrm{tr}[\gamma^\mu S(x,x'|A)\gamma^\nu S(x',x|A)]\,. \qquad (2.12)$$

The one-loop approximation used here neglects graphs containing more than one virtual photon, i.e., contributions to $W(T)$ of order e^4 are omitted. Therefore it is consistent to neglect terms of the same order in the computation of the trace under consideration. This is achieved in the following way: we write

$$-i\frac{\delta^2 S_{\text{eff}}}{\delta A_\nu(x')\,\delta A_\mu(x)}=K^{\mu\nu}(x,x')+L^{\mu\nu}(x,x')\,, \tag{2.13}$$

where

$$K^{\mu\nu}(x,x')=-i\,\Box g^{\mu\nu}\,\delta^4(x-x')=O(e^0)\,,$$

$$L^{\mu\nu}(x,x')=e^2\,\mathrm{tr}\,[\gamma^\mu S(x,x'\,|A)\gamma^\nu S(x',x\,|A)]=O(e^2)\,.$$

Then we use the expansion[21]

$$\ln(K+L)=\ln K+K^{-1}L+O(e^4)\,, \tag{2.14}$$

where K^{-1} is the photon propagator

$$K^{-1}_{\mu\nu}(x,x')=iD_{\mu\nu}(x-x')\,, \tag{2.15}$$

because

$$\Box_x D^\mu_\nu(x-x')=\delta^\mu_\nu\,\delta^4(x-x')\,; \tag{2.16}$$

$\mathrm{tr}\ln K$ is a constant determined by the spectrum of the d'Alembert operator. This constant is independent of A_μ and can be absorbed into the normalization constant N. We thus obtain

$$\begin{aligned}\mathrm{tr}\ln\left(-i\frac{\delta^2 S_{\text{eff}}}{\delta A_\nu\,\delta A_\mu}\,[a]\right)&=\mathrm{tr}\,K^{-1}L+O(e^4)\\&=ie^2\int d^4x\,d^4x'\,D_{\mu\nu}(x-x')\\&\quad\times\mathrm{tr}\,[\gamma^\nu S(x',x\,|A^{\text{cl}})\\&\quad\times\gamma^\mu S(x,x'\,|A^{\text{cl}})]+O(e^4)\,.\end{aligned} \tag{2.17}$$

In the case of a time-independent potential A^{ex}_μ, the propagator $S(x,x'\,|A^{\text{cl}})$ is a function of $\vec{x}$, $\vec{x}'$, and $x^0-x^{0\prime}$ only. This leads to

$$\begin{aligned}\mathrm{tr}\ln\left(-i\frac{\delta^2 S_{\text{eff}}}{\delta A_\nu\,\delta A_\mu}\,[a]\right)&=Tie^2\int d^3x\,d^4x'\,D_{\mu\nu}(x-x')\\&\quad\times\mathrm{tr}\,[\gamma^\nu S(x',x\,|A^{\text{cl}})\gamma^\mu S(x,x'\,|A^{\text{cl}})]+O(e^4)\,.\end{aligned} \tag{2.18}$$

The effective action at the stationary point is the sum of the "classical" field energy and a trace involving the Dirac operator:

$$\begin{aligned}S_{\text{eff}}[a]=\int_{t_1}^{t_2}dt\int d^3x\,(-\tfrac{1}{2}\partial_\mu a_\nu\partial^\mu a^\nu)\\-i\,\mathrm{tr}\ln\{-i[\gamma^\mu(i\partial_\mu-eA^{\text{cl}}_\mu)-m]\}\,.\end{aligned} \tag{2.19}$$

From Eqs. (2.8) and (2.16) we obtain for the potential $a_\mu(x)$

$$a^\mu(x)=-ie\int d^4x'\,D^{\mu\nu}(x-x')\,\mathrm{tr}\,[\gamma_\nu S(x',x'\,|A^{\text{cl}})]\,,$$

and the "classical" field energy can therefore be written as

$$\begin{aligned}&\int_{t_1}^{t_2}dt\int d^3x\,(-\tfrac{1}{2}\partial_\mu a_\nu\partial^\mu a^\nu)\\&\quad=-T\,\tfrac{1}{2}e^2\int d^3x\,d^4x'\,D^{\mu\nu}(x-x')\,\mathrm{tr}\,[\gamma_\mu S(x,x\,|A^{\text{cl}})]\\&\qquad\times\mathrm{tr}\,[\gamma_\nu S(x',x'\,|A^{\text{cl}})]\,.\end{aligned} \tag{2.20}$$

The computation of the trace occurring in (2.19) is more complicated and is explained in detail in Appendix A. Folowing Dashen *et al.*,[2] we obtain for large values of T

$$\begin{aligned}&-i\,\mathrm{tr}\ln\{-i[\gamma^\mu(i\partial_\mu-eA^{\text{cl}}_\mu)-m]\}\\&\quad=iT\int d^3x\;\mathrm{tr}\,[(-i\gamma^i\partial_i+m+e\gamma^\mu A^{\text{cl}}_\mu)S(x,y\,|A^{\text{cl}})]\big|_{y=x}\\&\quad=-T\sum_{n_<}\epsilon_n[A^{\text{cl}}]\,,\end{aligned} \tag{2.21}$$

where $\epsilon_n[A^{\text{cl}}]$ are the energies of the one-electron states in the potential A^{cl}_μ and the sum is over all negative-energy states.

Combining Eqs. (2.10) and (2.18)–(2.21), we obtain the result for $W(T)$ in the one-loop approximation, up to terms of order e^4 and for large values of T, and up to terms of order e^4,

$$\begin{aligned}W(T)=\exp\Big(&-iT\sum_{n_<}\epsilon_n[A^{\text{cl}}]+\tfrac{1}{2}e^2\int d^3x\,d^4x'\\&\times\{D^{\mu\nu}(x-x')\,\mathrm{tr}\,[\gamma_\mu S(x,x\,|A^{\text{cl}})]\,\mathrm{tr}\,[\gamma_\nu S(x',x'\,|A^{\text{cl}})]+D^{\mu\nu}(x-x')\,\mathrm{tr}\,[\gamma_\nu S(x',x\,|A^{\text{cl}})\gamma_\mu S(x,x'\,|A^{\text{cl}})]\}\Big)\,.\end{aligned} \tag{2.22}$$

For the energy of the vacuum in the potential A^{ex}_μ we thus obtain [cf. Eq. (2.5)]

$$E_{\text{vac}}[A^{\text{ex}}]=E_0[A^{\text{ex}}]+E_1[A^{\text{ex}}]\,,$$

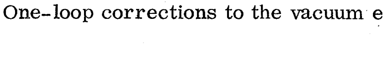

FIG. 1. One-loop corrections to the vacuum energy.

$$E_0[A^{\rm ex}]=\sum_{n_<} \epsilon_n[A^{\rm cl}]\,,$$

$$E_1[A^{\rm ex}]=\tfrac{1}{2}e^2\int d^3x\, d^4x'\, D^{\mu\nu}(x-x')$$
$$\times\{{\rm tr}\,[\gamma_\mu S(x,x\,|A^{\rm cl})]\,{\rm tr}\,[\gamma_\nu S(x',x'\,|A^{\rm cl})]$$
$$+{\rm tr}\,[\gamma_\nu S(x',x\,|A^{\rm cl})\gamma_\mu S(x,x'\,|A^{\rm cl})]\}\,.$$

The physical interpretation of this result is obvious: $E_0[A^{\rm ex}]$ is the energy of the "sea" of negative-energy states in the potential $A_\mu^{\rm cl}$ which are occupied according to Dirac's hole theory; $E_1[A^{\rm ex}]$ represents the sum of the lowest-order radiative corrections of the "sea" levels. These radiative corrections may be represented graphically as shown in Fig. 1. Using different techniques Dittrich has obtained the same result.[22]

III. TWO-ELECTRON STATES

Eqs. (2.23) and (2.21) show that the vacuum energy in an external potential is fully determined by the electron propagator in the field $A_\mu^{\rm cl}$. In this section I demonstrate how the presence of bound electrons may be taken into account by a substitution rule which modifies the electron-propagator. This substitution rule will be based on the Pauli principle, thus avoiding the self-interaction problem from the beginning.

We ask the question: how is the propagation of the virtual quanta modified by the presence of an additional bound electron? Let $\psi_1(t,\vec{x}),\psi_2(t',\vec{x})$ represent one-electron states at times t and t'. The amplitude for a transition between these two states under the influence of a potential $A_\mu^{\rm cl}$ is given by[23]

$$\langle 2,t'\,|S(A^{\rm cl})\,|1,t\rangle=\int d^3x\,\psi_2^\dagger(t',\vec{x})i\int d^3x'$$
$$\times S(t',\vec{x};t,\vec{x}'\,|A^{\rm cl})\gamma^0\psi_1(t,\vec{x}')\,. \quad (3.1)$$

For $t'>t$ the propagator can be written as

$$S(t',\vec{x}';t,\vec{x}\,|A^{\rm cl})=-i\sum_{n_>}\varphi_n(t',\vec{x}')\bar{\varphi}_n(t,\vec{x})\,, \quad (3.2)$$

where

$$\varphi_n(t,\vec{x})=\varphi_n(\vec{x})e^{-i\epsilon_n t} \quad (3.3)$$

are the eigenstates of the Dirac-operator in the potential $A_\mu^{\rm cl}$ and the sum is over all positive-energy states. The transition amplitude (3.1) therefore becomes

$$\langle 2,t'\,|S(A^{\rm cl})\,|1,t\rangle=\sum_{n_>}\int d^3x\,\psi_2^\dagger(t',\vec{x})\varphi_n(t',\vec{x})$$
$$\times\int d^3x'\,\varphi_n^\dagger(t,\vec{x}')\psi_1(t,\vec{x}') \quad (3.4)$$
$$=\sum_{n_>}\langle 2,t'\,|n,t'\rangle\langle n,t\,|t,1\rangle\,,$$

i.e., the transition $|1,\ t\rangle$ to $|2,\ t'\rangle$ may be visualized as a process taking place in two steps: at time t a transition from $|1\rangle$ to an intermediate state $|n\rangle$ occurs, followed by a second transition from $|n\rangle$ to $|2\rangle$ at time t'. To obtain the complete transition amplitude one must sum over all possible intermediate states.

How does the presence of a bound electron influence the transitions of the virtual quanta? One effect is that the virtual quanta now propagate in a potential $A_\mu^{\rm cl}$ which is generated by the current of the bound electron in addition to the external current. The second effect is due to the Pauli principle: the subspace being occupied by the bound electron cannot contribute to the transitions. Let $U(t,\vec{x})$ be the wave function of the additional electron. The transition amplitude then reads

$$\langle 2,t'\,|1,t\rangle_U$$
$$=\left\langle 2,t'\,\middle|\left(\sum_{n_>}|n,t'\rangle\langle n,t\,|-|U,t'\rangle\langle U,t\,|\right)\middle|1,t\right\rangle$$
$$=\langle 2,t'\,|S(A^{\rm cl}[U])\,|1,t\rangle-\langle 2,t'\,|U,t'\rangle\langle U,t\,|1,t\rangle\,.$$
$$(3.5)$$

The modification of the external potential as well as the change in the transition amplitude is obtained by the following substitution:

$$S(x,x'\,|A^{\rm cl})\to iU(x)\bar{U}(x')+S(x,x'\,|A^{\rm cl}[U])\,; \quad (3.6)$$

from Eq. (2.8) we obtain for the potential $A_\mu^{\rm cl}[U]$

$$\Box a_\mu(x\,|\,U)=e\bar{U}(x)\gamma_\mu U(x)$$
$$-ie\,{\rm tr}\,[\gamma_\mu S(x,x|A^{\rm cl}[U])]\,, \quad (3.7)$$
$$A_\mu^{\rm cl}[U]=A_\mu^{\rm ex}+a_\mu[U]\,.$$

For the transition amplitude the substitution (3.6) implies

$$\langle 2,t'\,|1,t\rangle_U$$
$$=\int d^3x\,\psi_2^\dagger(t',\vec{x})i\int d^3x'\,S(t',\vec{x};t,\vec{x}'\,|A^{\rm cl}[U])\gamma^0\psi_1(t,\vec{x}')-\int d^3x\,\psi_2^\dagger(t',\vec{x})U(t',\vec{x})\int d^3x'\,U^\dagger(t,\vec{x}')\psi_1(t,\vec{x}')$$
$$=\langle 2,t'\,|S(A^{\rm cl}[U])\,|1,t\rangle-\langle 2,t'\,|U,t'\rangle\langle U,t\,|1,t\rangle\,,$$

which is in agreement with Eq. (3.5).

To obtain the effect of two bound electrons on the propagation of the virtual quanta we employ the SCF picture. We approximate the two-electron state by a product of two one-electron states in some self-consistent field. Concerning the influence on the propagation of the virtual quanta, the two bound electrons therefore act completely independent, and instead of Eq. (3.6) we have the substitution rule

$$S(x,x'|A^{\mathrm{cl}}) \to iU_1(x)\overline{U}_1(x')+iU_2(x)\overline{U}_2(x') + S(x,x'|A^{\mathrm{cl}}[U_1,U_2]) , \qquad (3.8)$$

yielding for the potential $A_\mu^{\mathrm{cl}}[U_1,U_2]$

$$\Box a_\mu(x|U_1,U_2)=e\overline{U}_1(x)\gamma_\mu U_1(x)+e\overline{U}_2(x)\gamma_\mu U_2(x) -ie\,\mathrm{tr}\,[\gamma_\mu S(x,x|A^{\mathrm{cl}}[U_1,U_2])] , \qquad (3.9)$$

$$A_\mu^{\mathrm{cl}}[U_1,U_2]=A_\mu^{\mathrm{ex}}+a_\mu[U_1,U_2] ;$$

$U_1(x)$ and $U_2(x)$ are the wave functions of the bound electrons.

So far we have determined how the propagation of virtual quanta is changed by the presence of two bound electrons which, in the SCF approximation, are described by wave functions $U_1(x)$ and $U_2(x)$. We now employ this result to compute the energy of a two-electron state in the SCF approximation, taking one-loop quantum fluctuations into account. We achieve this by performing the substitution (3.8) in the vacuum energy which has been expressed in terms of the propagator $S(x,x'|A^{\mathrm{cl}})$ in Eqs. (2.23) and (2.21). The result is the following energy functional, dependent on the potential A_μ^{cl} and the wave functions $U_1(x)$ and $U_2(x)$:

$$\begin{aligned}E[A^{\mathrm{cl}};U_1,U_2] &= \sum_{i=1}^{2}\int d^3x\,\overline{U}_i(x)[-i\gamma^i\partial_i+m+e\gamma^\mu A_\mu^{\mathrm{ex}}(x)]U_i(x)+\sum_{i,j=1}^{2}\tfrac{1}{2}e^2\int d^3x\,d^4x'\,D^{\mu\nu}(x-x')[\overline{U}_i(x)\gamma_\mu U_i(x)\overline{U}_j(x')\gamma_\nu U_j(x')\\ &\quad -\overline{U}_i(x)\gamma_\mu U_j(x)\overline{U}_j(x')\gamma_\nu U_i(x')]+\sum_{i=1}^{2}e^2\int d^3x\,d^4x'\,\overline{U}_i(x)iD^{\mu\nu}(x-x')\gamma_\mu S(x,x'|A^{\mathrm{cl}})\gamma_\nu U_i(x')+\sum_{k_<}\epsilon_k[A^{\mathrm{cl}}]\\ &\quad +\tfrac{1}{2}e^2\int d^3x\,d^4x'\,D^{\mu\nu}(x-x')\{\mathrm{tr}[\gamma_\mu S(x,x|A^{\mathrm{cl}})]\mathrm{tr}[\gamma_\nu S(x',x'|A^{\mathrm{cl}})]+\mathrm{tr}\,[\gamma_\nu S(x',x|A^{\mathrm{cl}})\gamma_\mu S(x,x'|A^{\mathrm{cl}})]\} , \qquad (3.10)\end{aligned}$$

where the potential A_μ^{cl} is given by Eq. (3.9) (from now on I no longer indicate the dependence of A_μ^{cl} on U_1, U_2). The various terms in Eq. (3.10) have a familiar interpretation: the first two integrals are, apart from retardation effects, identical to the expectation value of the Hamiltonian employed in the ordinary relativistic Hartree-Fock ansatz[24]); the third term represents the well-known self-energy of the bound electrons, and the last two terms are the vacuum energy in the new field A_μ^{cl}.

In the treatment of bound states in quantum field theory one problem frequently encountered is the appearance of a classical self-interaction of the bound constituents. In the case of ordinary Fock-space methods this problem was discussed in detail in Ref. 16. The self-interaction problem can occur as well if one employs functional integral techniques, as I show in Appendix B. Owing to the presence of exchange terms the energy functional (3.10) does not contain self-interaction contributions, although in the course of the calculation leading to Eq. (3.10) various terms of this type occur. Surprisingly enough, however, the self-interaction terms arising from the one-loop part $E_1[A^{\mathrm{cl}}]$ of the vacuum energy cancel those from the "classical" part $E_0[A^{\mathrm{cl}}]$. To my mind this nontrivial cancellation is one of the strongest justifications for the postulated substitution (3.8) which is the basis of the approach presented here.

The wave functions $U_1(x)$ and $U_2(x)$ are unknown. According to the SCF picture we choose the time dependence to be

$$U_i(t,\vec{x})=U_i(\vec{x})\exp(-iE_it), \quad i=1,2 , \qquad (3.11)$$

where the one-particle energies E_i must be determined self-consistently. Then the direct interaction reads

$$\begin{aligned}I_{ij}^{D}&=\tfrac{1}{2}e^2\int d^3x\,d^4x'\,D^{\mu\nu}(x-x')\overline{U}_i(x)\gamma_\mu U_i(x)\times\overline{U}_j(x')\gamma_\nu U_j(x')\\ &=\frac{e^2}{8\pi}\int\frac{d^3x\,d^3x'}{|\vec{x}-\vec{x}'|}\overline{U}_i(\vec{x})\gamma^\mu U_i(\vec{x})\overline{U}_j(\vec{x}')\gamma_\mu U_j(\vec{x}') . \qquad (3.12)\end{aligned}$$

For the exchange terms we obtain

$$\begin{aligned}I_{ij}^{\mathrm{ex}}&=\tfrac{1}{2}e^2\int d^3x\,d^4x'\,D^{\mu\nu}(x-x')\overline{U}_i(x)\gamma_\mu U_j(x)\times\overline{U}_j(x')\gamma_\nu U_i(x')\\ &=\frac{e^2}{8\pi}\int\frac{d^3x\,d^3x'}{|\vec{x}-\vec{x}'|}\overline{U}_i(\vec{x})\gamma_\mu U_j(\vec{x})\times\overline{U}_j(\vec{x}')\gamma^\mu U_j(\vec{x}')\exp(i|E_i-E_j|\,|\vec{x}-\vec{x}'|) ; \qquad (3.13)\end{aligned}$$

when $E_i \neq E_j$ the exchange interaction thus receives a contribution from retardation. Taking terms up to order $(v/c)^2$ into account we arrive at[25]

$$I_{ij}^{\mathrm{ex}} = \frac{e^2}{8\pi}\int \frac{d^3x\,d^3x'}{|\vec{\mathrm{x}}-\vec{\mathrm{x}}'|}\Big(\overline{U}_i(\vec{\mathrm{x}})\gamma^0 U_j(\vec{\mathrm{x}})\overline{U}_j(\vec{\mathrm{x}}')\gamma^0 U_i(\vec{\mathrm{x}}') - \tfrac{1}{2}\overline{U}_i(\vec{\mathrm{x}})\gamma^k U_j(\vec{\mathrm{x}})\overline{U}_j(\vec{\mathrm{x}}')\gamma^k U_i(\vec{\mathrm{x}}')$$
$$- \frac{1}{2|\vec{\mathrm{x}}-\vec{\mathrm{x}}'|^2}\overline{U}_i(\vec{\mathrm{x}})\vec{\gamma}\cdot(\vec{\mathrm{x}}-\vec{\mathrm{x}}')U_j(\vec{\mathrm{x}})\overline{U}_j(\vec{\mathrm{x}}')\vec{\gamma}\cdot(\vec{\mathrm{x}}-\vec{\mathrm{x}}')U_i(\vec{\mathrm{x}}')\Big)\,. \tag{3.14}$$

The two-electron energy functional is therefore given by [c.f. (3.10)–(3.14)]

$$E[A^{\mathrm{cl}};U_1,U_2] = \sum_{i=1}^{2}\int d^3x\,\overline{U}_i(\vec{\mathrm{x}})[-i\gamma^i\partial_i + m + e\gamma_\mu A_\mu^{\mathrm{ex}}]U_i(\vec{\mathrm{x}}) + \frac{e^2}{4\pi}\int\frac{d^3x\,d^3x'}{|\vec{\mathrm{x}}-\vec{\mathrm{x}}'|}[\overline{U}_1(\vec{\mathrm{x}})\gamma^\mu U_1(\vec{\mathrm{x}})\overline{U}_2(\vec{\mathrm{x}}')\gamma^\mu U_2(\vec{\mathrm{x}}')$$
$$-\overline{U}_1(\vec{\mathrm{x}})\gamma^0 U_2(\vec{\mathrm{x}})\overline{U}_2(\vec{\mathrm{x}}')\gamma^0 U_1(\vec{\mathrm{x}}') + \tfrac{1}{2}\overline{U}_1(\vec{\mathrm{x}})\gamma^i U_2(\vec{\mathrm{x}})\overline{U}_2(\vec{\mathrm{x}}')\gamma^i U_1(\vec{\mathrm{x}}') + \tfrac{1}{2}\overline{U}_1(\vec{\mathrm{x}})\vec{\mathrm{n}}\cdot\vec{\gamma}U_2(\vec{\mathrm{x}})\overline{U}_2(\vec{\mathrm{x}}')\vec{\mathrm{n}}\cdot\vec{\gamma}U_1(\vec{\mathrm{x}}')]$$
$$+\sum_{i=1}^{2} e^2\int d^3x\,d^4x'\,\overline{U}_i(x)iD^{\mu\nu}(x-x')\gamma_\mu S(x,x'|A^{\mathrm{cl}})\gamma_\nu U_i(x') + E_{\mathrm{vac}}[A^{\mathrm{cl}}],\quad \vec{\mathrm{n}} = \frac{\vec{\mathrm{x}}-\vec{\mathrm{x}}'}{|\vec{\mathrm{x}}-\vec{\mathrm{x}}'|}\,. \tag{3.15}$$

Following the usual variational procedure the unknown spinors $U_1(\vec{\mathrm{x}})$ and $U_2(\vec{\mathrm{x}})$ are now determined by requiring them to form a stationary point of the functional (3.15):

$$\frac{\delta}{\delta\overline{U}_i(\vec{\mathrm{x}})}E[A^{\mathrm{cl}};U_1,U_2] = 0,\quad i=1,2\,. \tag{3.16}$$

As the wave functions represent states of unit charge, the variation must be restricted to functions satisfying

$$\int d^3x\,\overline{U}_i(\vec{\mathrm{x}})\gamma^0 U_i(\vec{\mathrm{x}}) = 1\,. \tag{3.17}$$

To evaluate the functional derivative of $E_{\mathrm{vac}}[A^{\mathrm{cl}}]$ we use Eqs. (2.23) and (2.21), as well as

$$\frac{\delta}{\delta A^\mu(x)}i\,\mathrm{tr}\ln\{i[\gamma^\mu(i\partial_\mu - eA_\mu) - m]\}$$
$$= -ie\,\mathrm{tr}[\gamma_\mu S(x,x|A)] \tag{3.18}$$

and

$$\frac{\delta A_\mu^{\mathrm{cl}}(x)}{\delta\overline{U}_i(\vec{\mathrm{x}}')} = \frac{e}{4\pi|\vec{\mathrm{x}}-\vec{\mathrm{x}}'|}\gamma_\mu U_i(\vec{\mathrm{x}}') - \frac{ie^2}{4\pi}\int\frac{d^3y}{|\vec{\mathrm{x}}-\vec{\mathrm{y}}|}\int d^4z$$
$$\times\,\mathrm{tr}[\gamma_\mu S(y,z|A^{\mathrm{cl}})\gamma^\nu S(z,y|A^{\mathrm{cl}})]\frac{\delta A_\nu^{\mathrm{cl}}(z)}{\delta\overline{U}_i(\vec{\mathrm{x}}')}\,. \tag{3.19}$$

As we have calculated the vacuum energy in the one-loop approximation only, we omit terms of the order e^4. The result is

$$\frac{\delta}{\delta\overline{U}_i(\vec{\mathrm{x}})}E_{\mathrm{vac}}[A^{\mathrm{cl}}]$$
$$= \frac{-ie^2}{4\pi}\gamma^\mu\Big(\int\frac{d^3x'}{|\vec{\mathrm{x}}-\vec{\mathrm{x}}'|}\,\mathrm{tr}[\gamma_\mu S(x',x'|A^{\mathrm{cl}}]\Big)U_i(\vec{\mathrm{x}})\,; \tag{3.20}$$

i.e., we obtain the vacuum polarization potential acting on the spinor $U_i(\vec{\mathrm{x}})$.

Using Eq. (3.20) we arrive from the extremum condition (3.16) at the following integro-differential equations:

$$\gamma^0[-i\gamma^i\partial_i + m + e\gamma^\mu A_\mu^{\mathrm{ex}}(\vec{\mathrm{x}}) + \frac{e^2}{4\pi}\gamma^\mu\int\frac{d^3x'}{|\vec{\mathrm{x}}-\vec{\mathrm{x}}'|}\overline{U}_j(\vec{\mathrm{x}}')\gamma_\mu U_j(\vec{\mathrm{x}}')]U_i(\vec{\mathrm{x}}) - \frac{e^2}{4\pi}\Big(\int\frac{d^3x'}{|\vec{\mathrm{x}}-\vec{\mathrm{x}}'|}\overline{U}_j(\vec{\mathrm{x}}')\gamma^0 U_i(\vec{\mathrm{x}}')\Big)U_j(\vec{\mathrm{x}})$$
$$+\frac{e^2}{8\pi}\gamma^0\gamma^i\Big(\int\frac{d^3x'}{|\vec{\mathrm{x}}-\vec{\mathrm{x}}'|}\overline{U}_j(\vec{\mathrm{x}}')\gamma^i U_i(\vec{\mathrm{x}}')\Big)U_j(\vec{\mathrm{x}}) + \frac{e^2}{8\pi}\gamma^0\vec{\mathrm{n}}\cdot\vec{\gamma}\Big(\int\frac{d^3x'}{|\vec{\mathrm{x}}-\vec{\mathrm{x}}'|}\overline{U}_j(\vec{\mathrm{x}}')\vec{\mathrm{n}}\cdot\vec{\gamma}U_i(\vec{\mathrm{x}}')\Big)U_j(\vec{\mathrm{x}})$$
$$+\int d^4x'\exp[iE_i(x_0 - x_0')]\gamma^0\sum(x,x'|A^{\mathrm{cl}})U_i(\vec{\mathrm{x}}') = E_iU_i(\vec{\mathrm{x}})\,, \tag{3.21}$$

where $i,j=1,2$, $i\neq j$, and

$$\sum(x,x'|A^{\mathrm{cl}}) = ie^2D^{\mu\nu}(x-x')\gamma_\mu S(x,x'|A^{\mathrm{cl}})\gamma_\nu - ie^2\gamma^\mu\delta^4(x-x')\int d^4x''\,D_{\mu\nu}(x'-x'')\,\mathrm{tr}[\gamma^\nu S(x'',x''|A^{\mathrm{cl}})]\,.$$

In Eqs. (3.21) the one-electron energies E_i, introduced in Eq. (3.11), appear as eigenvalues. They have been identified with the Lagrangian multipliers enforcing the normalization conditions (3.17). This identification is justified because in this way Eqs. (3.21) yield the Fock-Dirac equations in the nonrelativistic limit.[26]

The variational equations obtained are relativistic Hartree-Fock equations: each electron moves in the field generated by the external current as well as the other bound electron; in addition, retarded exchange forces and radiative corrections are taken into account.

It is interesting to consider the case that only one of the wave functions is different from zero. The variational equation for one bound electron reads

$$\gamma^0[-i\gamma^i\partial_i+m+e\gamma^\mu A_\mu^{\mathrm{ex}}(\vec{x})]U(x)+\int d^4x'\,\gamma^0\textstyle\sum(x,x'|A^{\mathrm{cl}})U(x')=EU(x)\,,$$
$$U(x)=U(\vec{x})\exp(-iEx_0)\,. \tag{3.22}$$

Equation (3.22) has the structure of Schwinger's equation,[27] which embodies the radiative corrections to the Dirac equation. The two equations differ, however, in the mass operator: $\sum(x,x'|A^{\mathrm{cl}})$ is the mass operator in the presence of the classical potential A_μ^{cl}, whereas in Schwinger's equation, the mass operator $\sum(x,x'|A^{\mathrm{ex}})$ in the external potential occurs. As A_μ^{cl} depends on $U(x)$ [cf. Eq. (3.9)], Eq. (3.22) is nonlinear! Such a nonlinearity would lead to an interesting new type of radiative correction, especially in the case of strong binding. The first nonlinear terms, however, are of order e^4. Contributions of this order were neglected when we calculated the vacuum energy in the one-loop approximation. It might well be that terms arising in the two-loop correction compensate the nonlinearities encountered in Eq. (3.22) in the same way as the self-energy contributions arising at the "classical" level are cancelled by terms from the one-loop correction. The radiative corrections in Eq. (3.22) have a meaning only up to order e^2, and in this order Eq. (3.22) and Schwinger's equation are identical.

IV. BOUND STATES WITH AN ARBITRARY NUMBER OF CONSTITUENTS

Generalization of the approach described in Sec. III to an arbitrary number of bound constituents is obvious. Let $U_i(x)$, $i=1,\ldots,N$, and $V_j(x)$, $j=1,\ldots,M$, be positive- and negative-energy spinors representing N electrons and M positrons in the SCF approximation. The substitution rule yielding the energy functional $E[A_\mu^{\mathrm{cl}};U_1,\ldots,V_M]$ then reads

$$S(x,x'|A^{\mathrm{cl}})\rightarrow i\sum_{i=1}^{N}U_i(x)\overline{U}_i(x')-i\sum_{j=1}^{M}V_j(x)\overline{V}_j(x')+S(x,x'|A^{\mathrm{cl}})\,, \tag{4.1}$$

where

$$U_i(x)=U_i(\vec{x})\exp(-iE_ix_0),\quad V_j(x)=V_j(\vec{x})\exp(iE_jx_0)\,. \tag{4.2}$$

The potential A_μ^{cl} is the solution of the differential equation obtained by applying the substitution (4.1) to Eq. (2.8):

$$\Box a_\mu(x)=e\sum_{i=1}^{N}\overline{U}_i(x)\gamma_\mu U_i(x)-e\sum_{j=1}^{M}\overline{V}_j(x)\gamma_\mu V_j(x)-ie\,\mathrm{tr}\,[\gamma_\mu S(x,x|A^{\mathrm{cl}})]\,, \tag{4.3}$$
$$A_\mu^{\mathrm{cl}}=A_\mu^{\mathrm{ex}}+a_\mu\,.$$

Applied to the vacuum energy $E_{\mathrm{vac}}[A^{\mathrm{ex}}]$[cf. Eqs. (2.23) and (2.21)], the substitution rule (4.1) leads to

$$\begin{aligned}
E[A^{\mathrm{cl}};U_1,\ldots,V_M]
&=\sum_{i=1}^{N}\int d^3x\,\overline{U}_i(x)[-i\gamma^i\partial_i+m+e\gamma^\mu A_\mu^{\mathrm{ex}}(x)]U_i(x)-\sum_{j=1}^{M}\int d^3x\,\overline{V}_j(x)[-i\gamma^i\partial_i+m+e\gamma^\mu A_\mu^{\mathrm{ex}}(x)]V_j(x)\\
&\quad+\tfrac{1}{2}e^2\int d^3x\,d^4x'\,D^{\mu\nu}(x-x')\Bigg(\sum_{i,j=1}^{N}[\overline{U}_i(x)\gamma_\mu U_i(x)\overline{U}_j(x')\gamma_\nu U_j(x')-\overline{U}_i(x)\gamma_\mu U_j(x)\overline{U}_j(x')\gamma_\nu U_i(x')]\\
&\qquad+\sum_{i,j=1}^{M}[\overline{V}_i(x)\gamma_\mu V_i(x)\overline{V}_j(x')\gamma_\nu V_j(x')-\overline{V}_i(x)\gamma_\mu V_j(x)\overline{V}_j(x')\gamma_\nu V_i(x')]\\
&\qquad-2\sum_{i=1}^{N}\sum_{j=1}^{M}[\overline{U}_i(x)\gamma_\mu U_i(x)\overline{V}_j(x')\gamma_\nu V_j(x')-\overline{U}_i(x)\gamma_\mu V_j(x)\overline{V}_j(x')\gamma_\nu U_i(x)]\Bigg)\\
&\quad+\sum_{i=1}^{N}e^2\int d^3x\,d^4x'\,\overline{U}_i(x)iD^{\mu\nu}(x-x')\gamma_\mu S(x,x'|A^{\mathrm{cl}})\gamma_\nu U_i(x')\\
&\quad-\sum_{j=1}^{M}e^2\int d^3x\,d^4x'\,\overline{V}_j(x)iD^{\mu\nu}(x-x')\gamma_\mu S(x,x'|A^{\mathrm{cl}})\gamma_\nu V_j(x')+\sum_{k_<}\epsilon_k[A^{\mathrm{cl}}]\\
&\quad+\tfrac{1}{2}e^2\int d^3x\,d^4x'\,D^{\mu\nu}(x-x')\{\mathrm{tr}\,[\gamma_\mu S(x,x|A^{\mathrm{cl}})]\ \mathrm{tr}\,[\gamma_\nu S(x',x'|A^{\mathrm{cl}})]+\mathrm{tr}\,[\gamma_\nu S(x',x|A^{\mathrm{cl}})\gamma_\mu S(x,x'|A^{\mathrm{cl}})]\}\,.
\end{aligned} \tag{4.4}$$

This result is very similar to the energy functional $E[A^{\mathrm{cl}}; U_1, U_2]$ obtained in Sec. III [cf. Eq. (3.10)].

Again we can carry out the integration over x_0' for the direct- and exchange-interaction terms and write down the variational equations for the spinors $U_i(\vec{x})$ and $V_j(\vec{x})$. The only new terms occuring in the energy functional $E[A^{\mathrm{cl}}; U_1, \ldots, V_M]$ compared to $E[A^{\mathrm{cl}}; U_1, U_2]$ are those which involve positive- and negative-energy spinors. For the direct interaction we have

$$\begin{aligned} I_{ij}^{D} &= \tfrac{1}{2} e^2 \int d^3x\, d^4x'\, D^{\mu\nu}(x-x') \bar{U}_i(x) \gamma_\mu U_i(x) \\ &\quad \times \bar{V}_j(x') \gamma_\nu V_j(x') \\ &= \frac{e^2}{8\pi} \int \frac{d^3x\, d^3x'}{|\vec{x}-\vec{x}'|} \bar{U}_i(\vec{x}) \gamma^\mu U_i(\vec{x}) \bar{V}_j(\vec{x}') \gamma_\mu V_j(\vec{x}') . \end{aligned} \tag{4.5}$$

The exchange-interaction terms are given by

$$\begin{aligned} I_{ij}^{\mathrm{ex}} &= \tfrac{1}{2} e^2 \int d^3x\, d^4x'\, D^{\mu\nu}(x-x') \bar{U}_i(x) \gamma_\mu V_j(x) \\ &\quad \times \bar{V}_j(x') \gamma_\nu U_i(x') \\ &= \frac{e^2}{8\pi} \int \frac{d^3x\, d^3x'}{|\vec{x}-\vec{x}'|} \bar{U}_i(\vec{x}) \gamma_\mu V_j(\vec{x}) \bar{V}_j(\vec{x}') \gamma^\mu U_i(\vec{x}') \\ &\quad \times \exp[i(E_i+E_j)|\vec{x}-\vec{x}'|] ; \end{aligned}$$

in the case of nonrelativistic binding, i.e., $E_i + E_j \approx 2m$, we obtain the usual point interaction[28]

$$I_{ij}^{\mathrm{ex}} = -\frac{e^2}{8m^2} \int d^3x\, \bar{U}_i(\vec{x}) \gamma^\mu V_j(\vec{x}) \bar{V}_j(\vec{x}) \gamma_\mu U_i(\vec{x}) . \tag{4.6}$$

Using Eqs. (3.12) and (3.13) as well as Eqs. (4.5) and (4.6) one can immediately write down the variational equations for the spinors $U_i(\vec{x}), \ldots, V_j(\vec{x})$ which follow from minimizing the functional (4.4). The result is completely analogous to Eqs. (3.21) derived in the two-electron case.

V. CALCULATION OF BOUND-STATE ENERGIES

This section is devoted to the question of how the results obtained so far may be used to calculate the energy spectrum of bound electrons. In order to keep the notation simple, we confine ourselves to two electrons bound in an external potential A_μ^{ex}. The energy functional may be split into four parts,

$$E[A^{\mathrm{cl}}; U_1, U_2] = \sum_{i=1}^{2} E_i^{D} + E_{12} + \sum_{i=1}^{2} E_i^{\mathrm{SE}} + E_{\mathrm{vac}}[A^{\mathrm{cl}}], \tag{5.1a}$$

the expectation values of the Dirac Hamiltonian

$$E_i^{D} = \int d^3x\, \bar{U}_i(\vec{x}) [-i\gamma^i \partial_i + m + e\gamma^\mu A_\mu^{\mathrm{ex}}(\vec{x})] U_i(\vec{x}) , \tag{5.1b}$$

the direct- and exchange-interaction terms

$$\begin{aligned} E_{12} &= e^2 \int d^3x\, d^4x'\, D^{\mu\nu}(x-x') [\bar{U}_1(x) \gamma_\mu U_1(x) \\ &\quad \times \bar{U}_2(x') \gamma_\nu U_2(x') - \bar{U}_1(x) \gamma_\mu U_2(x) \bar{U}_2(x') \gamma_\nu U_1(x')] , \end{aligned} \tag{5.1c}$$

the self-energy corrections

$$\begin{aligned} E_i^{\mathrm{SE}} &= e^2 \int d^3x\, d^4x'\, \bar{U}_i(x) i D^{\mu\nu}(x-x') \gamma_\mu \\ &\quad \times S(x, x' | A^{\mathrm{cl}}) \gamma_\nu U_i(x') , \end{aligned} \tag{5.1d}$$

and the vacuum energy in the potential A_μ^{cl}

$$\begin{aligned} E_{\mathrm{vac}}[A^{\mathrm{cl}}] &= -i \int d^3x\, \mathrm{tr}\{[-i\gamma^i \partial_i + m + e\gamma^\mu A_\mu^{\mathrm{cl}}(\vec{x})] S(x, y | A^{\mathrm{cl}})\} \big|_{y=x} \\ &\quad + \tfrac{1}{2} e^2 \int d^3x\, d^4x'\, D^{\mu\nu}(x-x') \{ \mathrm{tr}[\gamma_\mu S(x, x | A^{\mathrm{cl}})]\, \mathrm{tr}[\gamma_\nu S(x', x' | A^{\mathrm{cl}})] + \mathrm{tr}[\gamma_\nu S(x', x | A^{\mathrm{cl}}) \gamma_\mu S(x, x' | A^{\mathrm{cl}})] \} . \end{aligned} \tag{5.1e}$$

Because of Eq. (3.9) the potential A_μ^{cl} is given by

$$A_\mu^{\mathrm{cl}}(x) = A_\mu^{\mathrm{ex}}(x) + a_\mu(x) , \tag{5.2}$$

where

$$a_\mu(x) = e \int d^4x'\, D_{\mu\nu}(x-x') \left(\sum_{i=1}^{2} \bar{U}_i(x') \gamma^\nu U_i(x') - i\, \mathrm{tr}[\gamma^\nu S(x', x' | A^{\mathrm{cl}})] \right) .$$

We now expand the propagator $S(x, x' | A^{\mathrm{cl}})$ in powers of e^2:

$$\begin{aligned} S(x, x' | A^{\mathrm{cl}}) &= S(x, x' | A^{\mathrm{ex}}) \\ &\quad + e^2 \int d^4y\, S(x, y | A^{\mathrm{ex}}) \gamma_\mu a^\mu(y) S(y, x' | A^{\mathrm{ex}}) + \cdots \\ &= S(x, x' | A^{\mathrm{ex}}) + O(e^2) . \end{aligned} \tag{5.3}$$

Using Eq. (5.3), we obtain up to terms of order e^4, which are neglected in the one-loop approximation,

$$\begin{aligned} E_{\mathrm{vac}}[A^{\mathrm{cl}}] &= \sum_{i=1}^{2} (-ie^2) \int d^3x\, d^4x'\, \bar{U}_i(x) \gamma_\mu \\ &\quad \times U_i(x) D^{\mu\nu}(x-x')\, \mathrm{tr}[\gamma_\nu S(x', x' | A^{\mathrm{cl}})] \\ &\quad + E_{\mathrm{vac}}[A^{\mathrm{ex}}] ; \end{aligned} \tag{5.4}$$

$E_{\text{vac}}[A^{\text{ex}}]$ is the vacuum energy in the presence of the external current only [cf. Eq. (2.23)]. The experimentally observed total energy of the two-electron state reads

$$E[U_1, U_2] = E[A^{\text{cl}}; U_1, U_2] - E_{\text{vac}}[A^{\text{ex}}]\,. \tag{5.5}$$

From Eqs. (5.1) and (5.4) we obtain

$$E[U_1, U_2] = \sum_{i=1}^{2} E_i^D + E_{12} + \sum_{i=1}^{2} E_i^{\text{RC}}\,, \tag{5.6a}$$

where the radiative corrections E_i^{RC} are the expectation values of the mass operator in the external potential

$$E_i^{\text{RC}} = \int d^3x\, d^4x'\, \overline{U}_i(x) \Sigma(x, x' | A^{\text{ex}}) U_i(x')\,,$$

$$\begin{aligned} \Sigma(x, x' | A^{\text{ex}}) &= ie^2 D^{\mu\nu}(x - x')\gamma_\mu S(x, x' | A^{\text{ex}})\gamma_\nu - ie^2\gamma^\mu \delta^4(x - x') \\ &\quad \times \int d^4x''\, D_{\mu\nu}(x' - x'')\, \text{tr}\, [\gamma^\nu S(x'', x'' | A^{\text{ex}})]\,. \end{aligned} \tag{5.6b}$$

Neglecting again radiative corrections of order e^4 the variational equations determining the spinors $U_i(\vec{x})$ are [cf. Eqs. (3.21)]

$$\begin{aligned} &\gamma^0\left(-i\gamma^i\partial_i + m + e\gamma^\mu A_\mu^{\text{ex}}(\vec{x}) + \frac{e^2}{4\pi}\gamma^\mu \int \frac{d^3x'}{|\vec{x} - \vec{x}'|}\overline{U}_j(\vec{x}')\gamma_\mu U_j(\vec{x}')\right) U_i(\vec{x}) \\ &\qquad - e^2\gamma^0\gamma^\mu\left(\int d^4x'\, \exp[i(E_i - E_j)(x_0 - x_0')] D_{\mu\nu}(x - x')\overline{U}_j(\vec{x}')\gamma^\nu U_i(\vec{x}')\right) U_j(\vec{x}) \\ &\qquad + \int d^4x'\, \exp[iE_i(x_0 - x_0')]\gamma^0 \Sigma(x, x' | A^{\text{ex}}) U_i(\vec{x}') = E_i U_i(\vec{x})\,, \quad i, j = 1, 2,\ i \neq j\,. \end{aligned} \tag{5.7}$$

In terms of the eigenvalues E_i the total, experimentally observable energy of the two-electron state is given by

$$E[U_1, U_2] = E_1 + E_2 - e^2 \int d^3x\, d^4x'\, D^{\mu\nu}(x - x')[\overline{U}_1(x)\gamma_\mu U_1(x)\overline{U}_2(x')\gamma_\nu U_2(x') - \overline{U}_1(x)\gamma_\mu U_2(x)\overline{U}_2(x')\gamma_\nu U_1(x')]\,. \tag{5.8}$$

The relativistic Hartree-Fock equations (5.7) incorporate radiative corrections in the leading order. They are the simplest equations which might have been guessed: the single-particle radiative corrections described by Schwinger's equation[27] are simply added to the ordinary Hartree-Fock equations.

In principle there should be no difficulty in using Eqs. (5.7) for explicit calculations, although technically they will be very complicated. The renormalization of the mass operator is known from the single-particle case.[8,9] For weak external potentials one can treat the radiative corrections perturbatively, starting from a solution of the ordinary Hartree-Fock equations. In the case of strong potentials, however, the mass operator must be incorporated in the variational procedure.

The method employed to obtain Eqs. (5.7) can be extended to derive variational equations which include higher-order radiative corrections: one must go beyond the one-loop approximation for the vacuum energy before applying the substitution rule (3.8). Most probably the simple structure of Eqs. (5.7) will not survive, and in addition to higher-order contributions to the mass-operator radiative corrections of the direct- and exchange-interaction terms will occur.

SCF equations similar to Eqs. (5.7) have been obtained by Reinhard, Greiner, and Arenhövel[13] for one-electron states in an external potential; these equations were extended to variational equations for many-electron bound states by Rafelski, Müller, and Greiner.[14] The result obtained by these authors differs from Eqs. (5.7) in the treatment of the quantum corrections. Whereas in Ref. 14 bound electrons and negative-energy "sea" electrons are determined by the same SCF equations, Eqs. (5.7) involve the mass operator in the external potential only, i.e., the "sea" electrons obey simply the Dirac equation in the external potential. In the approach developed in the previous sections no recoupling of the "sea" to the bound electrons occurs in a consistent treatment at the level of one-loop radiative corrections.

VI. SUMMARY

Employing functional integration methods developed by Dashen *et al.*[2] and a new substitution rule, we have derived relativistic SCF equations which incorporate radiative effects. The substitution rule has been justified by the Pauli principle and the SCF picture. The obtained variational equations have a familar physical interpretation. Self-interaction terms do not occur and exchange-interactions are taken into account; single-particle radiative corrections have been added with respect to ordinary relativistic Hartree-Fock equations.

The basic problem of Hartree-Fock equations is the lack of a procedure allowing for the computation of corrections to the variational approximation in a systematic way. This leads to some arbitrariness of SCF equations. I find it interesting that the equations derived in Sec. IV contain retarded exchange interactions, while the direct interactions are instantaneous. Different SCF approaches may lead to different equations[16] yielding, for example, both interactions to be either instantaneous or retarded. As long as a systematic perturbation theory around Hartree-Fock equations does not exist it cannot be decided theoretically which interaction yields the most appropriate zeroth-order approximation.

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APPENDIX A

In Appendix A I calculate the trace needed in Sec. II [cf. Eq. (2.21)]. For a time-independent potential $A_\mu(\vec{x})$ the Dirac operator

$$\gamma^0(\not{D}-m)=\gamma^0[\gamma^\mu(i\partial_\mu-eA_\mu)-m] \tag{A1}$$

possesses a complete set of periodic eigenfunctions $\varphi_{n,m}(x)$:

$$\varphi_{n,m}(x)=\varphi_n(\vec{x})e^{-i\omega_m t},$$

$$\omega_m=2\pi m/T, \quad T=t_2-t_1, \quad m\in Z,$$

$$\int_{t_1}^{t_2}\int d^3x\,\varphi^\dagger_{n',m'}\varphi_{n,m}=\delta_{nn'}\delta_{mm'}, \tag{A2}$$

$$\int_{t_1}^{t_2}dt\int d^3x\,\varphi^\dagger_{n',m'}\gamma^0(\not{D}-m)\varphi_{n,m}$$

$$=(\omega_m-\epsilon_n)\delta_{nn'}\delta_{mm'},$$

where

$$\gamma^0[-i\gamma^k\partial_k+m+e\gamma^\mu A_\mu]\varphi_n=\epsilon_n\varphi_n. \tag{A3}$$

We thus obtain

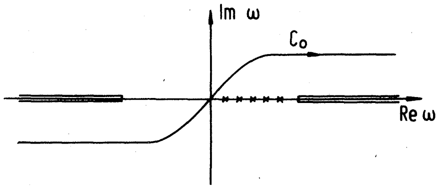

FIG. 2. Integration contour for the Feynman propagator.

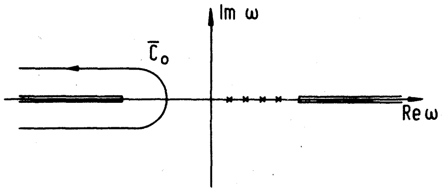

FIG. 3. Contour for the vacuum energy.

$$\operatorname{tr}\ln[-i(\not{D}-m)]=\operatorname{tr}\ln[-i\gamma^0(\not{D}-m)]$$

$$=\sum_{n,m}\ln[-i(\omega_m-\epsilon_n)]\underset{T\to\infty}{\to}\frac{T}{2\pi}\int_{-\infty}^{+\infty}d\omega$$

$$\times\sum_n\ln[-i(\omega-\epsilon_n)]. \tag{A4}$$

The Feynman boundary-conditions determine how the singularities occuring in Eq. (A4) must be circumvented. The spectral representation of the Feynman propagator reads (cf. Fig. 2)

$$S(x,x'|A)=\frac{1}{2\pi}\int_{C_0}d\omega\sum_n\frac{\varphi_n(\vec{x})\overline{\varphi}_n(\vec{x}')}{\omega-\epsilon_n}e^{-i\omega(t-t')}$$

$$=\frac{1}{2\pi}\int_{-\infty}^{+\infty}d\omega\sum_n\frac{\varphi_n(\vec{x})\overline{\varphi}_n(\vec{x}')}{\omega-\epsilon_n+i(\epsilon_n/|\epsilon_n|)\delta}e^{-i\omega(t-t')}, \tag{A5}$$

from which we infer

$$\operatorname{tr}\ln[-i(\not{D}-m)]$$

$$=\frac{T}{2\pi}\int_{-\infty}^{+\infty}d\omega\sum_n\ln[-i(\omega-\epsilon_n+i(\epsilon_n/|\epsilon_n|)\delta)]. \tag{A6}$$

An integration by parts[2] yields, up to a constant which can be absorbed in the normalization constant N occuring in Eq. (2.1),

$$\operatorname{tr}\ln[-i(\not{D}-m)]=-\frac{T}{2\pi}\int_{C_0}d\omega\sum_n\frac{\omega}{\omega-\epsilon_n}. \tag{A7}$$

Deforming the contour C_0 to encircle the negative-energy poles leads to the result quoted in Sec. II (cf. Fig. 3):

$$\operatorname{tr}\ln[-i(\not{D}-m)]=-\frac{T}{2\pi}\int_{\overline{C}_0}d\omega\sum_n\frac{\omega}{\omega-\epsilon_n}$$

$$=-iT\sum_{n_<}\epsilon_n.$$

Using Eqs. (A3) and (A5), we may express the trace as

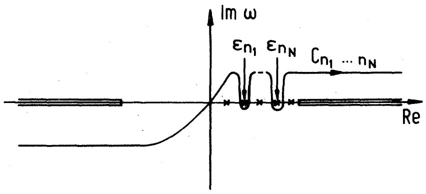

FIG. 4. Contour for an N-electron bound state.

$$\operatorname{tr}\ln[-i(\not{D}-m)] = -T\int d^3x\, \operatorname{tr}\left[(-i\gamma^i\partial_i + m + e\gamma^\mu A_\mu)S(x,y\,|A)\right]\Big|_{y=x}\,. \tag{A8}$$

APPENDIX B

The method employed by Dashen *et al.*[2] to derive variational equations for bound states proceeds as follows. The starting point is the effective action for static potentials $A_\mu(\vec{x})$ [cf. Eqs. (2.4)]. The effective action of an N-electron bound state is obtained by replacing the contour C_0 by $C_{n_1,\ldots,n_N}$ (cf. Fig. 4). The result for the energy of the N-electron state is

$$E_{n_1,\ldots,n_N}[A] = \tfrac{1}{2}\int d^3x\, \partial_i A_\mu \partial^i A^\mu + \sum_{i=1}^{N}\epsilon_{n_i} + \sum_{n_<}\epsilon_n\,. \tag{B1}$$

The energy levels ϵ_n are obtained as eigenvalues of the Dirac operator in a "classical" potential A_μ^{cl}

$$\gamma^0[-i\gamma^i\partial_i + m + e\gamma^\mu A_\mu^{\mathrm{cl}}]\varphi_n = \epsilon_n\varphi_n\,, \tag{B2}$$

which is determined by minimizing the energy functional (B1):

$$A_\mu^{\mathrm{cl}}(x) = A_\mu^{\mathrm{ex}}(x) + a_\mu(x)\,,$$

$$-\Delta a_\mu(x) = \sum_{i=1}^{N} e\overline{\varphi}_n(x)\gamma_\mu\varphi_n(x) - ie\,\operatorname{tr}\left[\gamma_\mu S(x,x\,|A^{\mathrm{cl}})\right]. \tag{B3}$$

Equations (B2) and (B3) are relativistic Hartree-Fock equations incorporating vacuum polarization effects. As is most easily seen in the case of one bound electron, they lead, however, to a classical self-interaction which is not experimentally observed in atomic spectra.

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