PHYSICAL REVIEW A VOLUME 18, NUMBER 5 NOVEMBER 1978

Variational approach to bound states in quantum electrodynamics

W. Buchmüller
Universität Bonn, Physikalisches Institut, D-5300 Bonn, Germany
(Received 3 March 1978)

A self-consistent-field approximation is employed to treat bound states in spinor electrodynamics. The proposed method avoids the classical self-interaction of bound quanta arising in variational approximations based on coherent trial states. Relativistic Hartree-Fock equations are obtained and implications for the calculation of atomic structures are discussed.

I. INTRODUCTION

In recent years variational approaches have frequently been employed to treat the bound-state problem in quantum field theory.[1] In particular using a semiclassical variational approximation Bardeen *et al.*[1] investigated in great detail the possibility of describing hadrons as bound states in a strongly coupled field theory. As it turned out, however, the quantum corrections to the semiclassical treatment are large and can not be treated economically as a perturbation in the strong-coupling case. Therefore the applicability of the approach of Bardeen *et al.* seems to be restricted to the weak-coupling regime.

In this paper we discuss a variational approach to bound states in quantum electrodynamics (QED), a weakly-coupled field theory. We do this for two reasons: firstly the variational approach to bound states in QED is interesting because of its applications to atomic physics; secondly the experimental and theoretical knowledge being available for QED provides a test for variational approximations. Indeed we find that the ansatz of Bardeen *et al.* which is based on a coherent trial state is not appropriate for the description of bound states in QED.

Existing atomic-structure calculations are mainly based on relativistic self-consistent-field (SCF) equations. Although there have been great improvements in the technique of handling these equations during the last years it is still an unsolved problem how to incorporate magnetic interactions and radiative effects in the self-consistent procedure.[2,3] This question is of particular importance in the case of heavy atoms where the Coulomb repulsion of the electrons, their magnetic interactions, and radiative effects are all of the same order of magnitude. It should be possible to answer this question by applying a SCF approximation to the bound-state problem in QED.

The paper is organized as follows: in Sec. II we present a variational ansatz for bound states in QED and derive the corresponding relativistic Hartree-Fock equations. In Sec. III these are applied to calculate the bound-state energy of heliumlike ions with large nuclear charge Z. The calculation employs an expansion in powers of $1/Z$. In particular the order of magnitude of terms arising in second-order perturbation theory is discussed. This leads to general implications for the calculation of atomic structures which we consider in Sec. V. Section IV deals with the variational approach employed by Bardeen *et al.* We conclude with a discussion of our results in Sec. VI.

II. VARIATIONAL METHOD

We will illustrate our variational approach to the bound-state problem for quantum electrodynamics in a time-independent external potential $A_\mu(\vec{x})$. Starting from the Lagrangian in the Feynman gauge[4]

$$\mathcal{L} = -\tfrac{1}{2}\partial_\mu A_\nu \partial^\mu A^\nu + \bar{\psi}[\gamma^\mu(i\partial_\mu - eA_\mu^{ex} - eA_\mu) - m]\psi \,, \tag{2.1}$$

the equations of motion are

$$[\gamma^\mu(i\partial_\mu - eA_\mu^{ex} - eA_\mu) - m]\psi = 0 \,, \tag{2.2a}$$

$$\Box A_\mu = e\bar{\psi}\gamma_\mu\psi \,. \tag{2.2b}$$

The theory is quantized by imposing equal-time commutation relations on the field operators at a fixed time which we take to be $t=0$. Adopting the Gupta-Bleuler formalism for the quantization of the vector field these commutation relations are

$$\{\psi_\alpha^\dagger(0,\vec{x}),\psi_\beta(0,\vec{x}')\} = \delta_{\alpha\beta}\delta(\vec{x}-\vec{x}') \,, \tag{2.3a}$$

$$[\overset{\circ}{A}_\mu(0,\vec{x}),A_\nu(0,\vec{x}')] = ig_{\mu\nu}\delta(\vec{x}-\vec{x}') \,. \tag{2.3b}$$

The Hamiltonian which generates the equations of motion (2.2) is

$$H=\int d^3x\{-\tfrac{1}{2}\dot{A}_\mu\dot{A}^\mu+\tfrac{1}{2}(\partial_i A_\mu)(\partial^i A^\mu) +\bar{\psi}[-i\gamma^i\partial_i+m+e\gamma^\mu A_\mu^{ex}+e\gamma^\mu A_\mu]\psi\}\ . \tag{2.4}$$

Our aim is to describe the bound state of electrons and positrons interacting with one another and with the external potential $A_\mu(\vec{x})$. Physically one expects that in the Hilbert space there exist eigenstates of the Hamiltonian corresponding to stable ground-state configurations and other states characterized by complex expectation values of the Hamiltonian and representing unstable excited configurations. As we are unable to construct these states explicity in a given Fock-space basis we are forced to use some approximation which we choose to be the self-consistent-field approximation. In addition we will neglect the interaction of the electrons and positrons with the radiation field; this implies that in our approximation excited states are placed on the same footing with ground states.

The SCF approximation is frequently used in nonrelativistic quantum mechanics.[5] There it means the approximation of an N-electron wave function $\phi(\vec{x}_1,\ldots,\vec{x}_N)$ by a single antisymmetrized product of N orthogonal functions $\phi_i(\vec{x}_i)$ $(i=1,\ldots,N)$, whereas the most general form of the wave function is a linear combination of all n-fold products of a complete orthonormal set of functions. The $\phi_i(\vec{x}_i)$'s are then determined by requiring them to be a stationary point of the expectation value of the Hamilton operator in the product state. This ansatz for the wave function is based on the following physical assumption: the interaction of the various bound quanta with one another and with the external potential can be represented by some self-consistent-field in which each constituent moves independently of the others.

This procedure can be applied to quantum field theory in a similar way. Let us consider a state $|N,M\rangle$ corresponding to a configuration of N electrons and M positrons. In the SCF picture they are represented by N spinors $U_n(\vec{x})$ and M spinors $V_m(\vec{x})$ which are positive and negative energy solutions of the Dirac equation in the self-consistent-field obeying the orthonormality relations

$$\int d^3x\bar{U}_n(\vec{x})\gamma^0U_m(\vec{x})=\int d^3x\,V_n(\vec{x})\gamma^0V_m(\vec{x})=\delta_{nm}\ ,$$
$$\int d^3x\,\bar{U}_n(\vec{x})\gamma^0V_m(\vec{x})=0\ . \tag{2.5}$$

The bound state $|N,M\rangle$ can then be generated by the creation operators

$$B_n^\dagger=\int d^3x\bar{\psi}(\vec{x})\gamma^0U_n(\vec{x})\ ,$$
$$D_m^\dagger=\int d^3x\bar{V}_m(\vec{x})\gamma^0\psi(\vec{x})\ , \tag{2.6}$$

which satisfy the canonical anticommutation relations

$$\{B_n,B_m^\dagger\}=\{D_n,D_m^\dagger\}=\delta_{nm}\ . \tag{2.7}$$

To obtain the bound states in the SCF approximation the creation operators $B_n^\dagger, D_m^\dagger$ have to operate on a no-particle state $|0\rangle$ which represents the vacuum in the self-consistent-field and which is defined by

$$B_n|0\rangle=D_m|0\rangle=0\ . \tag{2.8}$$

For the state $|N,M\rangle$ of N electrons and M positrons we can now write

$$|N,M\rangle=|n_1,\ldots,n_N;\bar{m}_1,\ldots,\bar{m}_M\rangle\otimes|A(N,M)\rangle\ ,$$
$$|n_1,\ldots,n_N;m_1,\ldots,m_M\rangle=B_{n_1}^\dagger\ldots B_{n_N}^\dagger D_{m_1}^\dagger\ldots D_{m_M}^\dagger|0\rangle\ , \tag{2.9}$$

where $|A(N,M)\rangle$ is a physical photon state representing the interaction between electrons and positrons. We assume this photon state to be completely determined by the fermion quantum numbers $n_1,\ldots,\bar{m}_M$.

The next step of the variational procedure is to calculate the expectation value of the Hamiltonian in the trial state (2.9). To do this it is not necessary to specify the photon state $|A(N,M)\rangle$ in terms of a given Fock-space basis. As we will show it is possible in the chosen approximation to reduce the expectation value of H to expectation values of products of the fermion field operator. In this way the dependence on the state $|A(N,M)\rangle$ disappears.

Integrating Eq. (2.2b) we obtain for the Hamiltonian

$$H=\int d^3x\{-\tfrac{1}{2}\dot{A}_\mu(\vec{x})\dot{A}^\mu(\vec{x})+\tfrac{1}{2}A_\mu(\vec{x})\ddot{A}^\mu(\vec{x})+\bar{\psi}(\vec{x})[-i\gamma^i\partial_i+m+e\gamma^\mu A_\mu^{ex}(\vec{x})]\psi(\vec{x})\}$$
$$+\frac{e^2}{8\pi}\int\frac{d^3x\,d^3x'}{|\vec{x}-\vec{x}'|}\,\bar{\psi}(\vec{x})\gamma^\mu\psi(\vec{x})[\bar{\psi}(\vec{x}')\gamma_\mu\psi(\vec{x}')-(1/e)\ddot{A}_\mu(\vec{x}')]\ . \tag{2.10}$$

Assuming $|N,M\rangle$ to represent an eigenstate of H we have

$$\langle N,M|\dot{A}_\mu(\vec{x})|N,M\rangle=\langle N,M|\ddot{A}_\mu(\vec{x})|N,M\rangle=0. \tag{2.11}$$

Expression (2.10) contains three terms involving time derivatives of the photon field. Because of Eq. (2.11) only "off-diagonal" intermediate states contribute to the expectation values of these terms with respect to $|N,M\rangle$. Therefore it is reasonable to neglect these contributions to the expectation value of H. This, of course, means to neglect contributions arising from the interaction of the bound quanta with the radiation field. One thus obtains

$$\langle N,M|H|N,M\rangle=\langle N,M|\int d^3x\,\bar{\psi}(\vec{x})[-i\gamma^i\partial_i+m+e\gamma^\mu A_\mu^{ex}(\vec{x})]\psi(\vec{x})+\frac{e^2}{8\pi}\int\frac{d^3x\,d^3x'}{|\vec{x}-\vec{x}'|}\bar{\psi}(\vec{x})\gamma^\mu\psi(\vec{x})\bar{\psi}(\vec{x}')\gamma_\mu\psi(\vec{x}')|N,M\rangle. \tag{2.12}$$

The right-hand side of Eq. (2.12) does not depend on the photon state $|A(N,M)\rangle$ and can be evaluated using Eqs. (2.3a) and (2.5)–(2.9). We assume the operator products occurring in Eq. (2.12) to be normal-ordered with respect to a basis of spinors including $U_{n_1}(\vec{x}),\ldots,V_{m_M}(\vec{x})$. The result is

$$\begin{aligned}\langle N,M|H|N,M\rangle=&\sum_{i=1}^{N}\int d^3x\,\bar{U}_{n_i}(\vec{x})[-i\gamma^i\partial_i+m+e\gamma^\mu A_\mu^{ex}(\vec{x})]U_{n_i}(\vec{x})\\&-\sum_{j=1}^{M}\int d^3x\,\bar{V}_{m_j}(\vec{x})[-i\gamma^i\partial_i+m+e\gamma^\mu A_\mu^{ex}(\vec{x})]V_{m_j}(\vec{x})\\&+\frac{e^2}{8\pi}\int\frac{d^3x\,d^3x'}{|\vec{x}-\vec{x}'|}\Bigg(\sum_{i,j=1}^{N}[\bar{U}_{n_i}(\vec{x})\gamma^\mu U_{n_i}(\vec{x})\bar{U}_{n_j}(\vec{x}')\gamma_\mu U_{n_j}(\vec{x}')-\bar{U}_{n_i}(\vec{x})\gamma^\mu U_{n_j}(\vec{x})\bar{U}_{n_j}(\vec{x}')\gamma_\mu U_{n_i}(\vec{x}')]\\&+\sum_{i,j=1}^{M}[V_{m_i}(\vec{x})\gamma^\mu V_{m_i}(\vec{x})\bar{V}_{m_j}(\vec{x}')\gamma_\mu V_{m_j}(\vec{x}')-\bar{V}_{m_i}(\vec{x})\gamma^\mu V_{m_j}(\vec{x})\bar{V}_{m_j}(\vec{x}')\gamma_\mu V_{m_i}(\vec{x}')]\\&-2\sum_{i=1}^{N}\sum_{j=1}^{M}[\bar{U}_{n_i}(\vec{x})\gamma^\mu U_{n_i}(\vec{x})\bar{V}_{m_j}(\vec{x}')\gamma_\mu V_{m_j}(\vec{x}')-\bar{U}_{n_i}(\vec{x})\gamma^\mu V_{m_j}(\vec{x})\bar{V}_{m_j}(\vec{x}')\gamma_\mu U_{n_i}(\vec{x}')]\Bigg).\end{aligned} \tag{2.13}$$

The spinors $U_{n_i}(\vec{x})$ and $V_{m_j}(\vec{x})$ are now determined by requiring them to form a stationary point of the functional $\langle N,M|H|N,M\rangle$. This leads to the variational equations

$$\begin{aligned}&\gamma^0\Bigg[-i\gamma^i\partial_i+m+e\gamma^\mu A_\mu^{ex}(\vec{x})+\frac{e^2}{4\pi}\gamma^\mu\int\frac{d^3x'}{|\vec{x}-\vec{x}'|}\Bigg(\sum_{j=1}^{N}\bar{U}_{n_j}(\vec{x}')\gamma_\mu U_{n_j}(\vec{x}')-\sum_{j=1}^{M}\bar{V}_{m_j}(\vec{x}')\gamma_\mu V_{m_j}(\vec{x}')\Bigg)\Bigg]U_{n_i}(\vec{x})\\&-\sum_{j=1}^{N}\frac{e^2}{4\pi}\gamma^0\gamma^\mu\Bigg(\int\frac{d^3x'}{|\vec{x}-\vec{x}'|}\bar{U}_{n_j}(\vec{x}')\gamma_\mu U_{n_i}(\vec{x}')\Bigg)U_{n_j}(\vec{x})+\sum_{j=1}^{M}\frac{e^2}{4\pi}\gamma^0\gamma^\mu\Bigg(\int\frac{d^3x'}{|\vec{x}-\vec{x}'|}\bar{V}_{m_j}(\vec{x}')\gamma_\mu U_{n_i}(\vec{x}')\Bigg)V_{m_j}(\vec{x})=E_{n_i}U_{n_i}(\vec{x}),\end{aligned} \tag{2.14}$$

$$\begin{aligned}&-\gamma^0\Bigg[-i\gamma^i\partial_i+m+e\gamma^\mu A_\mu^{ex}(\vec{x})+\frac{e^2}{4\pi}\gamma^\mu\int\frac{d^3x'}{|\vec{x}-\vec{x}'|}\Bigg(\sum_{j=1}^{N}\bar{U}_{n_j}(\vec{x}')\gamma_\mu U_{n_j}(\vec{x}')-\sum_{j=1}^{M}\bar{V}_{m_j}(\vec{x}')\gamma_\mu V_{m_j}(\vec{x}')\Bigg)\Bigg]V_{m_i}(\vec{x})\\&+\sum_{j=1}^{N}\frac{e^2}{4\pi}\gamma^0\gamma^\mu\Bigg(\int\frac{d^3x'}{|\vec{x}-\vec{x}'|}\bar{U}_{n_j}(\vec{x}')\gamma_\mu V_{m_i}(\vec{x}')\Bigg)U_{n_j}(\vec{x})-\sum_{j=1}^{M}\frac{e^2}{4\pi}\gamma^0\gamma^\mu\Bigg(\int\frac{d^3x'}{|\vec{x}-\vec{x}'|}\bar{V}_{m_j}(\vec{x}')\gamma_\mu V_{m_i}(\vec{x}')\Bigg)V_{m_j}(\vec{x})=E_{m_i}V_{m_i}(\vec{x}).\end{aligned} \tag{2.15}$$

The eigenvalues E_{n_i}, E_{m_j} appear as Lagrangian multipliers enforcing the normalization of the spinors. It is easy to check that for every solution of Eqs. (2.14) and (2.15) the spinors $U_{n_i}(\vec{x})$ and $V_{m_j}(\vec{x})$ are orthogonal to each other, i.e., the orthonormality relations (2.5) are fulfilled.

The obtained variational equations are relativistic Hartree-Fock equations: every particle moves in the field generated by the external charge and all the other bound quanta; in addition exchange forces appear. Equations (2.14) and (2.15) are similar to variational equations used for atomic-structure calculations. A detailed comparison will be given in Sec. V.

III. HELIUMLIKE IONS WITH LARGE Z

In this section we consider a simple application of the obtained Hartree-Fock equations. We will calculate relativistic corrections to the ground-state energy of heliumlike ions with large nuclear charge Z.

For large Z we can use the familiar expansion in powers of $1/Z$.[6] The results of this calculation will lead us to some general conclusions concerning the calculation of atomic structures which will be discussed in Sec. V. Choosing $N=2$, $M=0$, $A_\mu^{ex}(\vec{x})=(-Ze/4\pi r,\vec{0})$ we obtain from Eqs. (2.12) ($\alpha=e^2/4\pi, r=|\vec{x}|$)

$$\gamma^0\left(-i\gamma^i\partial_i+m-\frac{Z\alpha}{r}\gamma^0+\frac{1}{Z}(Z\alpha)\gamma^\mu\int\frac{d^3x'}{|\vec{x}-\vec{x}'|}\,\bar{U}_{n_2}(\vec{x}')\gamma_\mu U_{n_2}(\vec{x}')\right)U_{n_1}(\vec{x})$$
$$-\frac{1}{Z}(Z\alpha)\gamma^0\gamma^\mu\left(\int\frac{d^3x'}{|\vec{x}-\vec{x}'|}\,\bar{U}_{n_2}(\vec{x}')\gamma_\mu U_{n_1}(\vec{x}')\right)U_{n_2}(\vec{x})=E_{n_1}U_{n_1}(\vec{x}),\quad(3.1a)$$

$$\gamma^0\left(-i\gamma^i\partial_i+m-\frac{Z\alpha}{r}\gamma^0+\frac{1}{Z}(Z\alpha)\gamma^\mu\int\frac{d^3x'}{|\vec{x}-\vec{x}'|}\,\bar{U}_{n_1}(\vec{x}')\gamma_\mu U_{n_1}(\vec{x}')\right)U_{n_2}(\vec{x})$$
$$-\frac{1}{Z}(Z\alpha)\gamma^0\gamma^\mu\left(\int\frac{d^3x'}{|\vec{x}-\vec{x}'|}\,\bar{U}_{n_1}(\vec{x}')\gamma_\mu U_{n_2}(\vec{x}')\right)U_{n_1}(\vec{x})=E_{n_2}U_{n_2}(\vec{x}).\quad(3.1b)$$

The electron-electron interaction is suppressed by $1/Z$ with respect to the electron-nucleus interaction and one can therefore solve Eqs. (3.1) using perturbation theory. Wave functions and eigenvalues are expanded in powers of $1/Z$ ($i=1,2$):

$$U_{n_i}(\vec{x})=\phi_i^{(0)}(\vec{x})+(1/Z)\phi_i^{(1)}(\vec{x})+(1/Z)^2\phi_i^{(2)}(\vec{x})+\cdots,$$
$$E_{n_i}=\epsilon_i^{(0)}+(1/Z)\epsilon_i^{(1)}+(1/Z)^2\epsilon_i^{(2)}+\cdots.\quad(3.2)$$

Inserting the expansion (3.2) into Eq. (3.1a) one obtains up to order $(1/Z)^2$:

$$[\gamma^0(-i\gamma^i\partial_i+m)-Z\alpha/r-\epsilon_1^{(0)}]\,\phi_1^{(0)}=0,\quad(3.3a)$$

$$[\gamma^0(-i\gamma^i\partial_i+m)-Z\alpha/r-\epsilon_1^{(0)}]\phi_1^{(1)}+(Z\alpha)\gamma^0\gamma^\mu\left(\int\frac{d^3x'}{|\vec{x}-\vec{x}'|}\,\bar{\phi}_2^{(0)}\gamma_\mu\phi_2^{(0)}\right)\phi_1^{(0)}-(Z\alpha)\gamma^0\gamma^\mu\left(\int\frac{d^3x'}{|\vec{x}-\vec{x}'|}\,\bar{\phi}_2^{(0)}\gamma_\mu\phi_1^{(0)}\right)$$
$$\times\phi_2^{(0)}-\epsilon_1^{(1)}\phi_1^{(0)}=0,\quad(3.3b)$$

$$[\gamma^0(-i\gamma^i\partial_i+m)-Z\alpha/r-\epsilon_1^{(0)}]\,\phi_1^{(2)}+(Z\alpha)\gamma^0\gamma^\mu\left(\int\frac{d^3x'}{|\vec{x}-\vec{x}'|}\,\bar{\phi}_2^{(0)}\gamma_\mu\phi_2^{(0)}\right)\phi_1^{(1)}+(Z\alpha)\gamma^0\gamma^\mu\left(\int\frac{d^3x'}{|\vec{x}-\vec{x}'|}\,\bar{\phi}_2^{(0)}\gamma_\mu\phi_2^{(1)}+\bar{\phi}_2^{(1)}\gamma_\mu\phi_2^{(0)}\right)\phi_1^{(0)}$$
$$-(Z\alpha)\gamma^0\gamma^\mu\left(\int\frac{d^3x'}{|\vec{x}-\vec{x}'|}\,\bar{\phi}_2^{(0)}\gamma_\mu\phi_1^{(0)}\right)\phi_2^{(1)}-(Z\alpha)\gamma^0\gamma^\mu\left(\int\frac{d^3x'}{|\vec{x}-\vec{x}'|}\,\bar{\phi}_2^{(0)}\gamma_\mu\phi_1^{(1)}+\bar{\phi}_2^{(1)}\gamma_\mu\phi_1^{(0)}\right)\phi_2^{(0)}-\epsilon_1^{(1)}\phi_1^{(1)}-\epsilon_1^{(2)}\phi_1^{(0)}=0;\quad(3.3c)$$

interchanging the indices 1 and 2 in Eqs. (3.3) yields the analogous equations which follow from Eq. (3.1b). The orthonormality relations (2.5) imply up to order $(1/Z)^2$

$$\int d^3x\,\bar{\phi}_i^{(0)}\gamma^0\phi_j^{(0)}=\delta_{ij},\quad(3.4a)$$

$$\int d^3x(\bar{\phi}_i^{(0)}\gamma^0\phi_j^{(1)}+\bar{\phi}_i^{(1)}\gamma^0\phi_j^{(0)})=0,\quad(3.4b)$$

$$\int d^3x(\bar{\phi}_i^{(0)}\gamma^0\phi_j^{(2)}+\bar{\phi}_i^{(2)}\gamma^0\phi_j^{(0)}+\bar{\phi}_i^{(1)}\gamma^0\phi_j^{(1)})=0.\quad(3.4c)$$

In zeroth order Eqs. (3.1) reduce to the Dirac equation in a Coulomb potential. As we want to calculate the ground-state energy of heliumlike ions we have to choose the hydrogen ground-state wave function with spin up and down for $\phi_1^{(0)}$, $\phi_2^{(0)}$ (Ref. 4):

$$\phi_1^{(0)}(\vec{x})=\frac{(2mZ\alpha)^{3/2}}{\sqrt{4\pi}}\left(\frac{1+\gamma}{2\Gamma(1+2\gamma)}\right)^{1/2}$$
$$\times(2mZ\alpha r)^{\gamma-1}e^{-mZ\alpha r}$$
$$\times\begin{bmatrix}1\\0\\i\,\dfrac{1-\gamma}{Z\alpha}\cos\vartheta\\ i\,\dfrac{1-\gamma}{Z\alpha}\sin\vartheta e^{i\phi}\end{bmatrix},\quad(3.5)$$

$$\phi_2^{(0)}(\vec{x}) = \frac{(2mZ\alpha)^{3/2}}{\sqrt{4\pi}} \left(\frac{1+\gamma}{2\Gamma(1+2\gamma)}\right)^{1/2} \times (2mZ\alpha r)^{\gamma-1} e^{-mZ\alpha r} \times \begin{bmatrix} 0 \\ 1 \\ i\frac{1-\gamma}{Z\alpha}\sin\vartheta e^{-i\phi} \\ -i\frac{1-\gamma}{Z\alpha}\cos\vartheta \end{bmatrix}, \quad \gamma = [1-(Z\alpha)^2]^{1/2}.$$

The corresponding eigenvalues are

$$\epsilon_1^{(0)} = \epsilon_2^{(0)} = m[1-(Z\alpha)^2]^{1/2} = m[1 - \tfrac{1}{2}(Z\alpha)^2 - \tfrac{1}{8}(Z\alpha)^4 + O((Z\alpha)^6)]. \quad (3.6)$$

From Eqs. (3.3) one obtains for the first-order correction of the eigenvalues

$$\epsilon := \epsilon_1^{(1)} = \epsilon_2^{(1)} = Z\alpha \int \frac{d^3x d^3x'}{|\vec{x}-\vec{x}'|} (\bar{\phi}_2^{(0)}\gamma^\mu \phi_2^{(0)} \bar{\phi}_1^{(0)} \gamma_\mu \phi_1^{(0)} - \bar{\phi}_2^{(0)}\gamma^\mu \phi_1^{(0)} \bar{\phi}_1^{(0)} \gamma_\mu \phi_2^{(0)}). \quad (3.7)$$

The integral (3.7) may be split into four parts: a direct term and an exchange term both of which contain a Coulomb and a magnetic contribution. Using the wave functions (3.5) we obtain after some algebra

$$\epsilon = \epsilon_D^{\text{Coul}} + \epsilon_D^{\text{magn}} - \epsilon_{\text{ex}}^{\text{Coul}} - \epsilon_{\text{ex}}^{\text{magn}}, \quad (3.8a)$$

$$\epsilon_D^{\text{Coul}} = Z\alpha \int \frac{d^3x d^3x'}{|\vec{x}-\vec{x}'|} \bar{\phi}_2^{(0)}\gamma^\mu \phi_2^{(0)} \bar{\phi}_1^{(0)} \gamma_\mu \phi_1^{(0)} = \tfrac{5}{8} m(Z\alpha)^2 + \tfrac{3}{4}(1-\ln 2) m(Z\alpha)^4 + O((Z\alpha)^6), \quad (3.8b)$$

$$\epsilon_D^{\text{magn}} = Z\alpha \int \frac{d^3x d^3x'}{|\vec{x}-\vec{x}'|} \bar{\phi}_2^{(0)}\gamma^i \phi_2^{(0)} \bar{\phi}_1^{(0)} \gamma_i \phi_1^{(0)} = \tfrac{1}{6} m(Z\alpha)^4 + O((Z\alpha)^6), \quad (3.8c)$$

$$\epsilon_{\text{ex}}^{\text{Coul}} = Z\alpha \int \frac{d^3x d^3x'}{|\vec{x}-\vec{x}'|} \bar{\phi}_2^{(0)}\gamma^0 \phi_1^{(0)} \bar{\phi}_1^{(0)} \gamma^0 \phi_2^{(0)} = 0, \quad (3.8d)$$

$$\epsilon_{\text{ex}}^{\text{magn}} = Z\alpha \int \frac{d^3x d^3x'}{|\vec{x}-\vec{x}'|} \bar{\phi}_2^{(0)}\gamma^i \phi_1^{(0)} \bar{\phi}_1^{(0)} \gamma_i \phi_2^{(0)} = -\tfrac{1}{8} m(Z\alpha)^4 + O((Z\alpha)^6). \quad (3.8e)$$

For $Z < 1/\alpha$ the dominant contribution is given, of course, by the Coulomb repulsion of the electrons; this is the only part which contributes to the nonrelativistic binding energy. The Coulomb interaction as well as the magnetic interaction yield a relativistic correction proportional to $(Z\alpha)^4$ and one should note that all contributions are of the same order of magnitude.

From Eqs. (2.13), (3.1), (3.2), (3.6), and (3.8) we obtain for the total ground-state energy

$$E_G = E_{n_1} + E_{n_2} - \frac{1}{Z}(Z\alpha) \int \frac{d^3x d^3x'}{|\vec{x}-\vec{x}'|} (\bar{\phi}_2^{(0)}\gamma^\mu \phi_2^{(0)} \bar{\phi}_1^{(0)} \gamma_\mu \phi_1^{(0)} - \bar{\phi}_2^{(0)}\gamma^\mu \phi_1^{(0)} \bar{\phi}_1^{(0)} \gamma_\mu \phi_2^{(0)})$$

$$= m\{2 - (Z\alpha)^2[1 - \tfrac{5}{8}\tfrac{1}{Z} + O(1/Z^2)] - \tfrac{1}{4}(Z\alpha)^4[1 - (5 - 3\ln 2)\frac{1}{Z} + O(1/Z^2)] + O((Z\alpha)^6)\}. \quad (3.9)$$

This result is in good agreement with calculations using the Breit equation. The two approaches differ only on the term of order $(Z\alpha)^4$ $(1/Z)$. The Breit equation yields the coefficient 0.90 (Ref. 7) whereas Eq. (3.9) gives $\frac{1}{4}(5-3\ln 2) \approx 0.73$.

We now discuss the order of magnitude of the corrections in second-order perturbation theory. In accordance with Eq. (3.4b) we choose the functions $\phi_i^{(1)}$ orthogonal to $\phi_j^{(0)}$. Using Eqs. (3.3) this leads to

$$\epsilon_1^{(2)} = Z\alpha \int \frac{d^3x d^3x'}{|\vec{x}-\vec{x}'|} [\bar{\phi}_2^{(0)}\gamma^\mu \phi_2^{(0)} \bar{\phi}_1^{(0)} \gamma_\mu \phi_1^{(1)} + (\bar{\phi}_2^{(0)}\gamma^\mu \phi_2^{(1)} + \bar{\phi}_2^{(1)}\gamma^\mu \phi_2^{(0)}) \bar{\phi}_1^{(0)} \gamma_\mu \phi_1^{(0)} - \bar{\phi}_2^{(0)}\gamma^\mu \phi_1^{(0)} \bar{\phi}_1^{(0)} \gamma_\mu \phi_2^{(1)} - (\bar{\phi}_2^{(0)}\gamma^\mu \phi_1^{(1)} + \bar{\phi}_2^{(1)}\gamma^\mu \phi_1^{(0)}) \bar{\phi}_1^{(0)} \gamma_\mu \phi_2^{(0)}]. \quad (3.10)$$

Let $\{\psi_n\}$ denote those solutions of Eq. (3.3a) with positive and negative eigenvalues λ_n which are orthogonal to $\phi_i^{(0)}$. The functions $\phi_i^{(1)}$ may then be expressed as linear combinations of the ψ_n's where one has to sum over the discrete as well as the continuous part of the spectrum. From Eq. (3.3b), we obtain

$$\phi_i^{(1)}(\vec{x}) = \sum_n c_{in}\psi_n(mZ\alpha\vec{x}),$$

$$c_{in} = \frac{Z\alpha}{\epsilon_1^{(0)} - \lambda_n} \int \frac{d^3x\, d^3x'}{|\vec{x} - \vec{x}'|} (\bar{\phi}_2^{(0)}\gamma^\mu \phi_2^{(0)} \bar{\psi}_n \gamma_\mu \phi_1^{(0)} - \bar{\phi}_2^{(0)}\gamma^\mu \phi_1^{(0)} \bar{\psi}_n \gamma_\mu \phi_2^{(0)}),$$

$$c_{2n} = \frac{Z\alpha}{\epsilon_2^{(0)} - \lambda_n} \int \frac{d^3x\, d^3x'}{|\vec{x} - \vec{x}'|} (\bar{\phi}_1^{(0)}\gamma^\mu \phi_1^{(0)} \bar{\psi}_n \gamma_\mu \phi_2^{(0)} - \bar{\phi}_1^{(0)}\gamma^\mu \phi_2^{(0)} \bar{\psi}_n \gamma_\mu \phi_1^{(0)}). \tag{3.11}$$

Similar to Eqs. (3.8) one can split the functions $\phi_i^{(1)}$ into two parts $\phi_i^{(1)\,\mathrm{Coul}}$ and $\phi_i^{(1)\,\mathrm{magn}}$ one of which is determined by the Coulomb interaction while the other one is generated by the magnetic interaction. For $\epsilon_1^{(2)}$ we then obtain four contributions: the Coulomb part with the Coulomb correction of the wave functions $\phi_i^{(1)\,\mathrm{Coul}}$ ($\epsilon_1^{(2)\,\mathrm{Coul},\,\mathrm{Coul}}$), the Coulomb part with the magnetic wave-function corrections $\phi_i^{(1)\,\mathrm{magn}}$ ($\epsilon_1^{(2)\,\mathrm{Coul},\,\mathrm{magn}}$), the magnetic part with $\phi_i^{(1)\,\mathrm{Coul}}$ ($\epsilon_1^{(2)\,\mathrm{magn},\,\mathrm{Coul}}$) and the magnetic part with $\phi_i^{(1)\,\mathrm{magn}}$ ($\epsilon_1^{(2)\,\mathrm{magn},\,\mathrm{magn}}$).

For positive eigenvalues λ_n the lower components of the spinors ψ_n are suppressed by $Z\alpha$ with respect to the upper components, and the difference $\epsilon_i^{(0)} - \lambda_n$ is of the order $m(Z\alpha)^2$; for negative λ_n the upper components are smaller than the lower components by $Z\alpha$ and the difference $\epsilon_i^{(0)} - \lambda_n$ is of the order m. Using these properties of the wave functions[8] one easily finds that the four contributions to $\epsilon_1^{(2)}$ defined above are of the following order of magnitude:

$$\epsilon_1^{(2)\,\mathrm{Coul},\,\mathrm{Coul}} = O((Z\alpha)^2), \quad \epsilon_1^{(2)\,\mathrm{Coul},\,\mathrm{magn}} = O((Z\alpha)^4),$$
$$\epsilon_1^{(2)\,\mathrm{magn},\,\mathrm{Coul}} = O((Z\alpha)^4), \quad \epsilon_1^{(2)\,\mathrm{magn},\,\mathrm{magn}} = O((Z\alpha)^6). \tag{3.12}$$

The magnitude of the first and the third terms are as one may have expected. The contribution of the last term, a second-order magnetic correction, is smaller than the leading radiative correction yielding the Lamb shift which is of order $\alpha(Z\alpha)^4 \ln\alpha$. Therefore if one neglects radiative corrections one can calculate the ground-state energy systematically as a power series in $Z\alpha$ only up to order $(Z\alpha)^4$, and second-order magnetic corrections have no meaning as was pointed out by Bethe and Salpeter.[9] However, the second term in Eq. (3.12) shows that one is not allowed to neglect the magnetic corrections to the wave functions completely because these yield contributions to the energy of order $\alpha^2(Z\alpha)^2$. Further it is interesting to note that the contribution of wave functions with negative λ_n tp $\epsilon_1^{(2)}$ is of order $\alpha^2(Z\alpha)^4$ which again is negligible compared to radiative corrections.

IV. COHERENT-PHOTON TRIAL STATE

The variational approach to the bound-state problem in a strongly coupled field theory has been investigated in great detail by Bardeen *et al.*[1] The method described in Sec. II is similar to the procedure developed by these authors. There is, however, an essential difference. In Sec. II we avoided specifying the photon part of the trial state and preferred to reduce the problem to a self-interaction of the fermions. By way of contrast Bardeen *et al.* assume the quanta of the field producing the binding to be in a coherent state. As we will show this ansatz yields variational equations essentially different from Eqs. (2.14) and (2.15).

Let us expand the photon field in terms of plane waves

$$A_\mu(\vec{x}) = \frac{1}{(2\pi)^{3/2}} \int \frac{d^3k}{(2|\vec{k}|)^{1/2}} \times \sum_{\lambda=0}^{3} [a(\vec{k},\lambda)\epsilon_\mu(\vec{k},\lambda)e^{i\vec{k}\cdot\vec{x}} + a^\dagger(\vec{k},\lambda)\epsilon_\mu^*(\vec{k},\lambda)e^{-i\vec{k}\cdot\vec{x}}], \tag{4.1}$$

where

$$\epsilon_\mu^*(\vec{k},\lambda)\epsilon^\mu(\vec{k},\lambda') = \delta_{\lambda\lambda'}; \tag{4.2}$$

the operators $a(\vec{k},\lambda)$ and $a^\dagger(\vec{k},\lambda)$ satisfy canonical commutation relations

$$[a(\vec{k},\lambda),\, a^\dagger(\vec{k}',\lambda')] = -g_{\lambda\lambda'}\delta(\vec{k} - \vec{k}'). \tag{4.3}$$

Then the photon vacuum state $|\tilde{0}\rangle$ is characterized by

$$a(\vec{k},\lambda)|\tilde{0}\rangle = 0. \tag{4.4}$$

A coherent-photon state, parametrized by a classical field $a_\mu(\vec{x})$, is defined as

$$|a\rangle = \exp\left(i\int d^3x\, a^\mu(\vec{x})\dot{A}_\mu(\vec{x})\right)|\tilde{0}\rangle. \tag{4.5}$$

Requiring $|a\rangle$ to be a physical photon state, i.e.,

$$\partial_\mu A^{\mu(+)}(\vec{x})|a\rangle = 0\,, \tag{4.6}$$

yields the Lorentz condition for the field $a_\mu(\vec{x})$

$$\partial_\mu a^\mu(\vec{x}) = 0\,. \tag{4.7}$$

The ansatz of Bardeen *et al.* for a bound state of N electrons and M positrons is given by

$$|N, M; a\rangle = |n_1, \ldots, n_N; \bar{m}_1, \ldots, \bar{m}_M\rangle \otimes |a\rangle\,, \tag{4.8}$$

where the fermionic part of the trial state is unchanged with respect to Eq. (2.9).

The expectation value of the normal-ordered Hamiltonian (2.4) can easily be calculated. It is a functional of the spinors $U_n(\vec{x})$, $V_m(\vec{x})$, and the vector field $a_\mu(\vec{x})$:

$$\langle N,M;a|H|N,M;a\rangle = \int d^3x \Big(\tfrac{1}{2}\partial_i a_\mu(\vec{x})\partial^i a^\mu(\vec{x}) + \sum_{i=1}^{N} \bar{U}_{n_i}(\vec{x})[-i\gamma^i\partial_i + m + e\gamma^\mu A_\mu^{ex}(\vec{x}) + e\gamma^\mu a_\mu(\vec{x})]U_{n_i}(\vec{x})$$
$$- \sum_{j=1}^{M} \bar{V}_{m_j}(\vec{x})[-i\gamma^i\partial_i + m + e\gamma^\mu A_\mu^{ex}(\vec{x}) + e\gamma^\mu a_\mu(\vec{x})]V_{m_j}(\vec{x})\Big)\,. \tag{4.9}$$

Requiring the expectation value of the Hamiltonian to be a minimum with respect to all variations leaving the norm of the spinors invariant we obtain the variational equations

$$\gamma^0[-i\gamma^i\partial_i + m + e\gamma^\mu A_\mu^{ex}(\vec{x}) + e\gamma^\mu a_\mu(\vec{x})]U_{n_i}(\vec{x}) = E_{n_i}U_{n_i}(\vec{x})\,, \tag{4.10a}$$

$$-\gamma^0[-i\gamma^i\partial_i + m + e\gamma^\mu A_\mu^{ex}(\vec{x}) + e\gamma^\mu a_\mu(\vec{x})]V_{m_j}(\vec{x}) = E_{m_j}V_{m_j}(\vec{x})\,, \tag{4.10b}$$

$$-\Delta a_\mu(\vec{x}) = \sum_{i=1}^{N} e\bar{U}_{m_i}(\vec{x})\gamma_\mu U_{n_i}(\vec{x}) - \sum_{j=1}^{M} e\bar{V}_{m_j}(\vec{x})\gamma_\mu V_{m_j}(\vec{x})\,. \tag{4.10c}$$

Integrating Eq. (4.10c) yields

$$\gamma^0\Big[-i\gamma^i\partial^i + m + e\gamma^\mu A_\mu^{ex} + \frac{e^2}{4\pi}\gamma^\mu \int \frac{d^3x'}{|\vec{x}-\vec{x}'|}\Big(\sum_{i=1}^{N}\bar{U}_{n_i}\gamma_\mu U_{n_i} - \sum_{j=1}^{M}\bar{V}_{m_j}\gamma_\mu V_{m_j}\Big)\Big]U_{n_i} = E_{n_i}U_{n_i}\,, \tag{4.11}$$

$$-\gamma^0\Big[-i\gamma^i\partial^i + m + e\gamma^\mu A_\mu^{ex} + \frac{e^2}{4\pi}\gamma^\mu \int \frac{d^3x'}{|\vec{x}-\vec{x}'|}\Big(\sum_{i=1}^{N}\bar{U}_{n_i}\gamma_\mu U_{n_i} - \sum_{j=1}^{M}\bar{V}_{m_j}\gamma_\mu V_{m_j}\Big)\Big]V_{m_j} = E_{m_j}V_{m_j}\,. \tag{4.12}$$

In contrast to Eqs. (2.14) and (2.15) the variational equations (4.11) and (4.12) do not contain exchange terms. In some cases this can be a reasonable approximation. In the same way the Fock equations are often replaced by Hartree's equations in nonrelativistic quantum mechanics. Equations (4.11) and (4.12), however, do not just neglect exchange forces, in addition they give rise to a classical self-interaction of the bound fermions which is not observed in nature. This becomes most obvious in the case of one single electron bound in an external field. Choosing $N=1$, $M=0$ Eq. (4.11) reads

$$\gamma^0\Big(-i\gamma^i\partial_i + m + e\gamma^\mu A_\mu^{ex}(\vec{x}) + \frac{e^2}{4\pi}\int \frac{d^3x'}{|\vec{x}-\vec{x}'|}\bar{U}_n(\vec{x}')\gamma_\mu U_n(\vec{x}')\Big)U_n(\vec{x}) = E_n U_n(\vec{x})\,. \tag{4.13}$$

For an external Coulomb field, for instance, Eq. (4.13) does not even yield the correct nonrelativistic binding energies.

The problem of a classical self-interation of the matter-field quanta is typical for the treatment of bound states in field theory. It was first discussed in 1927 and 1928 by Jordan and Klein[10] and by Hartree.[11] Hartree simply omitted the self-coupling contributions; Jordan and Klein eliminated these terms by a normal-ordering prescription.

Because of the appearance of the classical self-interaction terms we conclude that coherent trial states are not appropriate for the description of bound states in weakly couplied field theories.

V. ATOMIC-STRUCTURE CALCULATIONS

Restricting ourselves to the case of N electrons moving in the Coulomb potential of a nucleus Eqs. (2.14) yield

$$\gamma^0\left(-i\gamma^i\partial_i+m-\frac{Z\alpha}{r}+\alpha\gamma^\mu\int\frac{d^3x'}{|\vec{x}-\vec{x}'|}\sum_{j=1}^{N}\bar{U}_{n_j}(\vec{x}')\gamma_\mu U_{n_j}(\vec{x}')\right)U_{n_i}(\vec{x})$$
$$-\alpha\sum_{j=1}^{N}\gamma^0\gamma^\mu\left(\int\frac{d^3x'}{|\vec{x}-\vec{x}'|}\bar{U}_{n_j}(\vec{x}')\gamma_\mu U_{n_i}(\vec{x}')\right)U_{n_j}(\vec{x})=E_{n_i}U_{n_i}(\vec{x})\ . \quad (5.1)$$

Equations (5.1) are similar to relativistic Hartree-Fock equations used for atomic-structure calculations.[12] Indeed they follow from the variational principle by choosing for the wave function a Slater determinant of Dirac spinors and by assuming the Hamilton operator of the N-electron system to be

$$H=\sum_{i=1}^{N}\left(-i\vec{\alpha}_{(i)}\vec{\nabla}_{(i)}+\beta_{(i)}m-\frac{Z\alpha}{r_i}\right)$$
$$+\frac{\alpha}{2}\sum_{i\neq j}\frac{1-\vec{\alpha}_{(i)}\cdot\vec{\alpha}_{(j)}}{|\vec{x}_i-\vec{x}_j|}\ ; \quad (5.2)$$

$\vec{\alpha}_{(i)}:=(\gamma^0\vec{\gamma})_{(i)}$ and $\beta_{(i)}:=\gamma^0{}_{(i)}$ act on the spinor $\psi_{n_i}(\vec{x}_i)$ of the Slater determinant.

Recent relativistic calculations of atomic structures are based on equations which differ from Eqs. (5.1) in two respects. The first difference concerns a simplification adopted for actual calculations. Instead of the unrestricted Hartree-Fock scheme yielding equations of the type (5.1) one uses a restricted Hartree-Fock scheme, i.e., one fixes the angular dependence of the spinors in the Slater determinant and solves variational equations for the radial wave functions only. The second difference lies in the choice of the electron-electron interaction Hamiltonian. For the magnetic part the Breit-Hamiltonian is employed so that the total interaction between two electrons i and j is given by

$$H_{ij}=H_{ij}^{\mathrm{Coul}}+H_{ij}^{\mathrm{magn}}+H_{ij}^{\mathrm{ret}}\ , \quad (5.3a)$$

$$H_{ij}^{\mathrm{Coul}}=\alpha/|\vec{x}_i-\vec{x}_j|\ , \quad (5.3b)$$

$$H_{ij}^{\mathrm{magn}}=-\frac{\alpha}{|x_i-x_j|}\vec{\alpha}_{(i)}\cdot\vec{\alpha}_{(j)}\ , \quad (5.3c)$$

$$H_{ij}^{\mathrm{ret}}=\frac{\alpha}{2|\vec{x}_i-\vec{x}_j|}\times\left(\vec{\alpha}_{(i)}\cdot\vec{\alpha}_{(j)}-\frac{[\vec{\alpha}_{(i)}\cdot(\vec{x}_i-\vec{x}_j)][\vec{\alpha}_{(j)}\cdot(\vec{x}_i-\vec{x}_j)]}{|\vec{x}_i-\vec{x}_j|^2}\right)\cdot \quad (5.3d)$$

H_{ij}^{Coul} and H_{ij}^{magn} correspond to the electrostatic and the magnetostatic interaction between the electrons; H_{ij}^{ret} represents the retardation effect of the electromagnetic interaction to leading order in an expansion in powers of $Z\alpha$. The correct way to compute relativistic binding energies is assumed to be the following: firstly wave functions and eigenvalues are determined from the variational equations containing the Coulomb interaction H_{ij}^{Coul} only; in a second step the expectation values of H_{ij}^{magn} and H_{ij}^{ret} are calculated to obtain the total energy. In this way the Breit interaction is treated in first-order perturbation theory only. To include it in the self-consistent procedure is claimed to be incorrect.[3,13]

By way of contrast Eqs. (5.1) neglect the retardation part of the interaction and include the magnetic part in the self-consistent procedure. The absence of a retardation term is not too surprising. The SCF method is a static approximation and applying it to field theory should only yield the static part of the interaction. In the SCF approximation for the wave function employing the static part of H_{ij} only could even yield a better estimate of binding energies than using the total Hamiltonian being inconsistent with the physical picture of the approximation. The question which interaction Hamiltonian should be used can only be answered by a numerical analysis.

The rule not to include the magnetic interaction in the self-consistent procedure is generally justified by the work of Bethe and Salpeter who observed that second-order magnetic corrections are inconsistent with a perturbation theory based on quantum electrodynamics.[9] This is in agreement with the result of Sec. III showing second-order magnetic contributions to be of order $\alpha^2(Z\alpha)^4$; calculcating binding energies systematically as power series in $Z\alpha$ these corrections have no meaning when radiative effects are neglected. In a numerical calculation, however, there is no reason—except for simplicity—to omit higher-order magnetic corrections because even in lowest order the binding energies are infinite power series in $Z\alpha$. In addition, as shown in Sec. III, not to include the magnetic interaction in the calculation of the wave functions means to neglect contributions to the energy of order $\alpha^2(Z\alpha)^2$ which can be large compared to radiative corrections which are of order $\alpha(Z\alpha)^4\ln\alpha$. We therefore conclude that one has to consider the magnetic interaction in the self-consistent procedure as is the case in Eqs. (5.1).

VI. DISCUSSION

We have considered variational approximations to the bound state problem in quantum electrodynamics. The variational approach based on a coherent-photon trial state is not appropriate because it gives rise to an unphysical classical self-interaction of the bound constituents. The SCF approximation presented in Sec. II avoids this problem and takes exchange forces into account.

The obtained relativistic SCF equations include the magnetic interaction of the bound electrons which is not the case in Hartree-Fock equations used so far in atomic-structure calculations. This leads to magnetic corrections of the wave functions. The calculation of the ground-state energy of heliumlike ions demonstrates the importance of these corrections as emphasized in Sec. V.

For very heavy atoms radiative effects are as important as the electro- and magnetostatic interactions. It remains to show how to include radiative effects in the self-consistent procedure. This problem can be solved using more complicated techniques. Dashen, Hasslacher, and Neveu have obtained bound-state equations of Hartree-Fock type in a two-dimensional-model field theory employing functional integration methods.[14] In a similar way the functional integral can be used to derive equations describing bound states in quantum electrodynamics which include radiative effects.[15] The results will be presented in a forthcoming publication.

ACKNOWLEDGMENTS

I would like to thank K. Dietz and E. Remiddi for clarifying discussions and K. Dietz also for a critical reading of the manuscript.

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