enological Lagrangian to study β decay. From the invariance of the Lagrangian under the given chiral symmetry or non-Abelian gauge group, a Noether's theorem is used to define physical current densities whose various T-products describe the decay process. However, these currents are derived by a Noether's theorem based on c-number variation techniques. In fact, Adler and Dashen[27] list at least two basic hypotheses in their monograph on current algebras which rest upon the c-number Noether's theorem techniques and as such do not consider any factor-ordering problems that might be present in these nonlinear, non-Abelian gauge theories.

Note added in proof. Equation (2.13) is also the necessary and sufficient condition for the nucleon current density $J^{\mu}(x)_a$ to satisfy the covariant conservation law $\nabla_{\mu} \cdot J^{\mu}(x) = 0$.

[27] S. L. Adler and R. F. Dashen, *Current Algebras and Applications to Particle Physics* (Benjamin, New York, 1968).

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Hartree-Fock Approximation in Quantum Electrodynamics

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A new approach to the bound-state problem in the frame of quantum electrodynamics is proposed, with special emphasis on the electron-proton bound states. It is an alternative approach to the usual one, which is based on the Bethe-Salpeter equation, and does not contain the ambiguities and unfamiliar features inherent in the Bethe-Salpeter theory. This approach is based on a straightforward generalization to quantum electrodynamics of the well-known Hartree-Fock approximation for the nonrelativistic theory of many-electron atoms.

I. INTRODUCTION

IT is well known that at the beginning of the last decade Bethe and Salpeter[1,2] (BS) suggested a fully covariant equation for the description of two interacting particles. In contrast to previous approaches, which introduced the nonrelativistic concept of instantaneous potentials to account for one of the particles, BS considered the relativistic retarded interaction between the particles. The BS approach was based on the intuitive Feynman-diagramatic techniques, and it was shown soon afterwards[3] that the equation could be derived more rigorously by using basic concepts of quantum field theory. Nevertheless, as stressed in Ref. 4 for example, so far it has not been possible to prove whether or not the BS equation provides in fact an exact solution corresponding to a realistic physical situation. Furthermore, the difficulties inherent in the BS equation were apparent from the beginning.[5,6] A significant simplification is obtained, however, if self-energy effects are removed from the equation. In terms of Feynman diagrams, this approximation is equivalent to the sum of only ladder diagrams, but, as shown by Cutkosky,[6] in the limit when the mass of one of the particles becomes infinite, the ladder approximation gives an equation which does not correspond to the motion of a particle in the field of a fixed center of force.[7–11] It seems therefore that from the ladder approximation alone we cannot expect to obtain, for example, the exact energy shift or the linewidth of two-body bound states.[12,13]

We propose in this paper an alternative approach that does not contain the unfamiliar features and ambiguities of the BS equation.[5,6,8] In contrast to the single BS equation we obtain a system of two coupled equations which, as will be shown, contain the main effects arising from the interaction between the particles. This system of two coupled integrodifferential equations for two particles is actually a simple and natural generalization, of the well-known Hartree-Fock (HF) equations in the familiar theory of nonrelativistic many-electron atoms. We are only interested here in the special case when $N=2$, where N is the total number of particles.[14] More precisely, we shall only consider

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[1] H. A. Bethe and E. E. Salpeter, Phys. Rev. **84**, 1232 (1951).
[2] J. Schwinger, Proc. Natl. Acad. Sci. (U.S.) **37**, 452 (1951).
[3] M. Gell-Mann and F. Low, Phys. Rev. **84**, 350 (1951).
[4] M. Günther, J. Math. Phys. **5**, 188 (1964).
[5] G. C. Wick, Phys. Rev. **96**, 1124 (1954).
[6] R. E. Cutkosky, Phys. Rev. **96**, 1135 (1954).
[7] Actually most of the subsequent investigations on the BS equation refer to the ladder approximation (see Refs. 5, 6, and 8–10).
[8] J. S. Goldstein, Phys. Rev. **91**, 1516 (1953).
[9] F. L. Scarf, Phys. Rev. **100**, 912 (1955).
[10] S. N. Biswas and H. S. Green, Nucl. Phys. **2**, 177 (1957).
[11] G. R. Allcok, Phys. Rev. **104**, 1799 (1956).
[12] S. S. Schweber, *An Introduction to Relativistic Quantum Field Theory* (Harper & Row, New York, 1961).
[13] E. A. Power, *Introductory Quantum Electrodynamics* (Green, London, 1964).
[14] In the ordinary HF theory the HF approximation is applied to a system of identical particles, i.e., to electrons in many-electron atoms (or molecules), and nucleons in many-nucleon nuclei. Here we shall study the relativistic bound states of nonidentical particles as, for example, the relativistic hydrogen atom.

here, in an explicit way, the case of two distinguishable particles. Instead of using in this generalization the instantaneous potential to describe the interaction, we shall consider the appropriate intermediate particles which mediate the interaction, i.e., photons for electromagnetic interactions and mesons for strong interactions. This fact, and the fact that in this generalization we do not include any external one-particle potential (which assures the existence of many-particle bound states), means that we shall not have a proper self-consistent potential nor proper stationary HF states, but unstable ones as it should be. The external potential appears in the nonrelativistic HF theory of many-electron atoms as the bare attractive Coulomb interaction between the atomic nucleus and atomic electrons. In the standard HF theory the initial external potential is transformed into a realistic self-consistent field which includes also the interaction among the electrons. This is an average potential acting on one electron, due to the nucleus and the remaining electrons.

In the theory we intend to develop here, the self-consistent potential does not contain an initial external field and therefore arises purely from the HF approximation to the attractive interaction between two particles.

In order to show that our generalized HF approximation can really describe bound states, let us consider the instructive example of the nonrelativistic hydrogen atom. Let $\psi_{e,p}(x)$ be the HF wave functions for an electron and proton, respectively. Then the HF self-consistent field acting on the electron due to the proton is given by

$$U_p(\mathbf{x})=\int \phi(|\mathbf{x}-\mathbf{x}'|)\psi_e^*(\mathbf{x}')\psi_e(\mathbf{x}')d^3x', \qquad (1.1)$$

where $\phi(|\mathbf{x}-\mathbf{x}'|)=-e^2/|\mathbf{x}-\mathbf{x}'|$ is the attractive Coulomb potential between the particles.

Similarly, the self-consistent potential acting on the proton due to the electron is

$$U_e(\mathbf{x})=\int \phi(|\mathbf{x}-\mathbf{x}'|)\psi_p^*(x')\psi_p(x')d^3x'. \qquad (1.2)$$

Now using Eqs. (1.1) and (1.2), we may write the corresponding Schrödinger equations

$$\begin{aligned} &-\frac{h^2}{2m_e}\nabla^2\psi_e(\mathbf{x})+U_p(\mathbf{x})\psi_e(\mathbf{x})=E_e\psi_e(\mathbf{x}),\\ &-\frac{h^2}{2m_p}\nabla^2\psi_p(\mathbf{x})+U_e(\mathbf{x})\psi_p(\mathbf{x})=E_p\psi_p(\mathbf{x}), \end{aligned} \qquad (1.3)$$

which correspond to the approximate Hartree equations. For $m_e/m_p\ll 1$ it is of course possible to neglect the quantum-mechanical effects on protons and simply drop out the last equation altogether. Thus, for an infinitely massive and localized proton we have, to a very good approximation,

$$\rho_p(\mathbf{x})=\psi_p^*(\mathbf{x})\psi_p(\mathbf{x})=\delta(\mathbf{x}), \qquad (1.4)$$

and Eqs. (1.3) reduce to the single equation

$$-\frac{h^2}{2m_e}\nabla^2\psi_e(\mathbf{x})-\frac{e}{|\mathbf{x}|}\psi_e(\mathbf{x})=E_e\psi_e(\mathbf{x}), \qquad (1.5)$$

i.e., the ordinary Schrödinger equation for hydrogen.

Notice that in the HF approximation just considered, the full two-body wave function has the structure $\psi(\mathbf{x}_1,\mathbf{x}_2)=\psi_e(\mathbf{x}_1)\psi_p(\mathbf{x}_2)$. This wave function is not of course an eigenstate of the total momentum, but an approximate eigenstate of the c.m. coordinate operator. This approximation is quite correct in the limit when the mass of one of the particles is infinite, i.e., when $m_e/m_p=0$. To calculate the full corrections due to the finite mass of the proton (i.e., when m_e is replaced by the reduced mass of the system), it is necessary to take into account the so-called correlation effects which are not included in the HF approximation.

We infer, therefore, that the HF approximation for a system of two interacting particles with attractive forces accounts in fact for the bound states of the system. In addition it should be stressed that we began with a self-consistent field which does not include at all some initial external potential.

It has been shown in the nonrelativistic theory[15] that the HF equations are mathematically equivalent to the sum of various Feynman diagrams, constructed exclusively with self-energy parts of first order.[16] This Feynman-diagramatic interpretation of the HF equations in the nonrelativistic theory with instantaneous two-particle interaction paves the way to generalize the HF equations for the case when the interaction is mediated by other particles.

In Appendix A we discuss the interpretation of the nonrelativistic HF equations in terms of Feynman diagrams.

In Sec. II, we extend to the relativistic domain the Feynman diagrams contained in the HF approximation and derive the equations that lead to these diagrams. We call these equations relativistic HF equations for hydrogen.[17–21]

[15] V. Tolmachev, Vestn. Leningr. Univ. Ser. Fiz. i Khim **N4** 11 (1962).

[16] In quantum electrodynamics, these self-energy parts of the first order correspond actually to second-order perturbation theory.

[17] We stress here the point that these are not the relativistic HF equations which appear in the literature (see Refs. 18–21). Our equations are expressed in terms of the retarded interaction between the particles in contrast with the ordinary relativistic HF equations, which involve static potentials and correspond therefore to the semirelativistic approach to the two-body problem.

[18] I. P. Grant, Proc. Roy. Soc. (London) **A262**, 555 (1961).

[19] G. L. Malli and C. C. J. Roothaan, Bull. Am. Phys. Soc. **9**, 101 (1964).

[20] M. Synek, Phys. Rev. **133**, A961 (1964).

[21] S. Fraga and G. Malli, *Many-Electron System Properties and Interactions* (Saunders, Philadelphia, 1968).

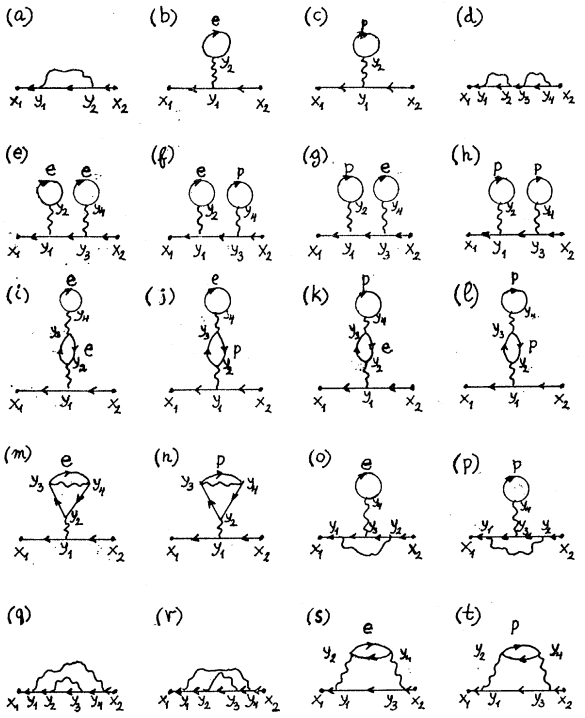

FIG. 1. Second- and fourth-order relativistic Feynman diagrams for one-particle propagators.

In Sec. III we consider the Hartree approximation to the relativistic HF equations for hydrogen, to obtain a system of equations which reduce in the nonrelativistic limit to Eqs. (1.3). When the proton is assumed to have infinite mass, both equations lead to a single Dirac equation for an electron in the presence of an instaneous Coulomb field. Making use of these results, we prove next that the relativistic HF equations for hydrogen yield the proper results for the energy shift and linewidth of the bound states. Finally we define two amplitudes for the electron and proton which play the role of wave functions, and derive the equations that are satisfied by these amplitudes.

II. RELATIVISTIC HF EQUATIONS

To obtain the relativistic HF equations, we shall follow the derivation of these equations in the nonrelativistic theory of many-electron atoms (see Appendix A). In order to fix the ideas, let us assume that the system is formed by an electron and a proton and consider only the bound states of the system. Our initial state will be, in ordinary second-quantization representation, one whose occupation numbers are one electron of momentum q^0 and one proton of momentum p^0. We shall denote this state by $|q^0p^0\rangle=|q^0\rangle|p^0\rangle$. The particles do not interact in zero approximation, i.e., both satisfy the free Dirac equation,

$$(i\gamma^\mu\partial_\mu-m_{e,p})\psi_{e,p}(x)=0, \tag{2.1}$$

and are described by plane waves of momentum q^0 and p^0, respectively. Notice that the Hamiltonian $H=H_0+H_{\text{int}}$ contains, in addition to the electron field, the proton-antiproton field. Our state $|q^0p^0\rangle$ belongs to the invariant subspace of H_0 with $N_e=1$ and $N_p=1$, where N_e is the number of electrons and N_p is the number of protons. We also point out that all our propagators will be defined in terms of this state rather than the vacuum state.

We define now the one-particle propagator for electrons and protons in the following way:

$$\langle p^0q^0|T\{\psi^{e,p}(x)\bar{\psi}^{e,p}(x)\}|q^0p^0\rangle\equiv-\tfrac{1}{2}S_F{}^{e,p}(x-x'), \tag{2.2}$$

which can be expressed in terms of the vacuum propagator as follows:

$$-\tfrac{1}{2}S_F{}^{e,p}(x-x')=-\tfrac{1}{2}S_F{}^{0e,p}(x-x')$$
$$-\frac{1}{(2\pi)^3}\frac{m_{e,p}}{E_{e,p}}\bar{\omega}_{e,p}{}^{(r)}\omega_{e,p}{}^{(r)}e^{-ip^0e,p(x-x')}\theta(x'-x), \tag{2.3}$$

where

$$S_F{}^{0e,p}(x-x')=\frac{1}{(2\pi)^3}\int\frac{d^3p}{2E_p}(\not{p}+m_{e,p})e^{-ip\cdot(x-x')}\theta(x-x')$$
$$-\frac{1}{(2\pi)^3}\int\frac{d^3q}{2E_p}(\not{p}-m_{e,p})e^{ip\cdot(x-x')}\theta(x'-x).$$

$\bar{\omega}_{e,p}{}^{(r)}(p)$ and $\omega_{e,p}{}^{(r)}(p)$ are free Dirac four-spinors, and r refers to the spin of the initial electron and proton. It is simple to prove that (2.3) reduces to (A6) in the nonrelativistic limit.

We notice here the difference between the one-particle propagator S_F and the ordinary Feynman or vacuum propagator $S_F{}^0$: in addition to $S_F{}^0$, S_F has an electron (proton) state of momentum q^0 (p^0) which like all positron (antiproton) states vanishes for $x_0'>x_0$ [see Eq. (2.3)]. Nevertheless, it is a genuine electron (proton) state corresponding to a positive-energy solution of the Dirac equation, or to positive-frequency part of second-quantized fields.

Using Eq. (2.3), it is simple to prove that the free one-particle propagator $S_F{}^{e,p}$, like the ordinary Feynman propagator $S_F{}^{0e,p}$, is a Green's function of Eq. (2.1), i.e., $S_F{}^{e,p}$ satisfies

$$(i\gamma^\mu\partial_\mu-m_{e,p})S_F{}^{e,p}(x-x')=-2i\delta^{(4)}(x-x'). \tag{2.4}$$

Let us now construct the Green's functions for the interacting particles and the corresponding Feynman diagrams. To do this we express the propagators in the interaction representation and apply to them the standard Dyson-Wick procedure. We obtain

$$\lim_{\alpha\to+0}\frac{\langle p^0q^0|T\{\psi(x)\bar{\psi}(x')S_\alpha(+\infty,-\infty)\}|q^0p^0\rangle}{\langle S_\alpha(+\infty,-\infty)\rangle}$$
$$=\langle p^0q^0|T\{\psi(x)\bar{\psi}(x')\}|q^0p^0\rangle, \tag{2.5}$$

where

$$S_\alpha(+\infty,-\infty)=\sum_{n=0}^{+\infty}\frac{(-i)^n}{n!}\int\cdots\int d^4y_1\cdots d^4y_n \times T\{\mathcal{H}_I(y_1)\cdots\mathcal{H}(y_n)\}e^{-\alpha(|y_1^0|+\cdots+|y_n^0|)} \quad (2.5')$$

and

$$\mathcal{H}_I(x)=eN\{\bar\psi_e(x)a(x)\psi_e(x)+\bar\psi_p(x)a(x)\psi_p(x)\}. \quad (2.5'')$$

The normal-ordered product in (2.5'') has been introduced in order to symmetrize the theory with respect to positrons and antiprotons.

The denominator which appears in Eq. (2.5) has the effect of excluding from the perturbation expansion of the numerator all vacuum diagrams (i.e., diagrams without external lines) as in the ordinary theory. Thus, for example, we obtain for the electron propagator, up to the fourth order of perturbation theory, all the Feynman diagrams shown in Fig. 1.

All electron and proton propagators which appear in Fig. 1 are one-particle propagators (otherwise some of them would be zero, namely, those which contain equal-time contractions). In other words, we have applied Wick's theorem in Eq. (2.5) for one-particle states rather than for the vacuum state. In Appendix B, we show how this can be justified. We only show here that equal-time contractions give rise to nonzero diagrams.

To do this, we have to consider terms like $N\{\bar\psi(x)\psi(x)\}$ which can also be written in the following form:

$$N\{\bar\psi(x)\psi(x)\}=\lim_{\epsilon\to+0}T\{\bar\psi(\xi)\psi(\xi)\}, \quad (2.6)$$

where

$$\psi(\xi)=\psi^{(+)}(\mathbf{x},x^0-\epsilon)+\psi^{(-)}(\mathbf{x},x^0+\epsilon),$$
$$\bar\psi(\xi)=\bar\psi^{(+)}(\mathbf{x},x^0-\epsilon)+\bar\psi^{(-)}(\mathbf{x},x^0+\epsilon). \quad (2.6')$$

The plus and minus signs in (2.6') refer to the positive- and negative-frequency parts of the wave operators.

For equal-time contractions we have, on account of Eq. (2.6), the following relation:

$$\langle p^0q^0|\,T\{N(\bar\psi(x)\psi(x))\}\,|q^0p^0\rangle = \lim_{\epsilon\to+0}\langle p^0q^0|\,T\{\bar\psi(\xi)\psi(\xi)\}\,|q^0p^0\rangle, \quad (2.7)$$

which, by using Eq. (2.3), reduces to

$$\langle p^0q^0|\,T\{N(\bar\psi(x)\psi(x))\}\,|q^0p^0\rangle = \lim_{\epsilon\to+0}\tfrac{1}{2}S_F{}^0(-\epsilon)+\lim_{\epsilon\to+0}\frac{1}{(2\pi)^3}\frac{m}{E}\times\bar\omega^{(r)}\omega^{(r)}e^{-ip^0\cdot\epsilon}\theta(\epsilon). \quad (2.8)$$

But $\lim_{\epsilon\to+0}S_F{}^0(-\epsilon)=0$ and therefore

$$\langle p^0q^0|\,T\{N(\bar\psi(x)\psi(x))\}\,|q^0p^0\rangle=\frac{1}{(2\pi)^3}\frac{m}{E}\bar\omega^{(r)}\omega^{(r)}. \quad (2.9)$$

We notice that in second order the same diagrams appear that yield the nonrelativistic HF equations. However, the propagator (2.5) contains, in higher orders of perturbation theory, diagrams which do not appear in the HF equations, and consequently we drop them. For example, in fourth order we neglect the last three diagrams (r)–(t) of Fig. 1. Thus, from all the diagrams contained in (2.5) we preserve only those which in the nonrelativistic limit yield the HF equations. Hence the one-particle propagator (2.5) will contain only the diagrams shown in Fig. 2. These diagrams correspond in fact to the nonrelativistic HF equations (see Appendix A).

The one-particle proton propagator is obtained by replacing, in Fig. 2, all electron lines by proton lines and vice versa, as indicated in the figure.

We notice here that instead of adding to the interaction Hamiltonian a term of the form $\delta m_eN(\bar\psi_e\psi_e)+\delta m_pN(\bar\psi_p\psi_p)$ in order to dress the initial particles, we assume that all our particles are physical ones. Hence we neglect the infinities arising from self-energy (or renormalization) diagrams and consider only their finite contributions. Otherwise we must include the diagrams arising from the renormalization factor just mentioned.

If we call $-\frac{1}{2}S_{F\mathrm{HF}}{}^{e,p}$ the approximate HF Green's functions of Fig. 2, we see that they satisfy the following nonlinear integral equation:

$$\begin{aligned}-\tfrac{1}{2}S_{F\mathrm{HF}}{}^{e,p}(x_1,x_2) &= -\tfrac{1}{2}S_F{}^{e,p}(x_1-x_2)-\frac{e^2}{2^4}\int\int S_F{}^{e,p}(x_1-y_1)\gamma^\mu\mathfrak{D}_F(y_1-y_2)\,\mathrm{Tr}(\gamma_\mu S_{F\mathrm{HF}}{}^{p,e}(y_2,y_1))S_{F\mathrm{HF}}{}^{e,p}(y_2x_2)d^4y_1d^4y_2\\ &\quad-\frac{e^2}{2^4}\int\int S_F{}^{e,p}(x_1-y_1)\gamma^\mu\mathfrak{D}_F(y_1-y_2)\,\mathrm{Tr}(\gamma_\mu S_{F\mathrm{HF}}{}^{e,p}(y_2,y_2))S_{F\mathrm{HF}}{}^{e,p}(y_1,x_2)d^4y_1d^4y_2\\ &\quad-\frac{e^2}{2^4}\int\int S_F{}^{e,p}(x_1-y_1)\gamma^\mu\mathfrak{D}_F(y_1-y_2)S_{F\mathrm{HF}}{}^{e,p}(y_1,y_1)\gamma_\mu S_{F\mathrm{HF}}{}^{e,p}(y_2,x_2)d^4y_1d^4y_2, \quad (2.10)\end{aligned}$$

where $\mathfrak{D}_F(x-x')$ is the usual Feynman photon propagator

$$\langle 0|\,P\{A_\mu(x)A_\nu(x')\}\,|0\rangle=-\tfrac{1}{2}g_{\mu\nu}\mathfrak{D}_F(x-x').$$

The system of the two coupled equations (2.10) constitutes the relativistic HF equations. We would like to point out that Eqs. (2.10) contain explicitly the scattering states only. In Sec. III, after rearranging these equations, we shall obtain in an explicit way the corresponding equations for the description of the bound states associated with the scattering states of Eqs. (2.10).

III. HARTREE APPROXIMATION TO HF EQUATIONS AND DIFFERENTIAL FORM OF RELATIVISTIC HF EQUATIONS

In order to obtain the Hartree approximation to the HF equations, we define a new propagator by rewriting Eqs. (2.10) in the following way:

$$-\tfrac{1}{2}S_{F\mathrm{HF}}{}^{e,p}(x_1,x_2)$$

$$=-\tfrac{1}{2}S_{F\mathrm{H}}{}^{e,p}(x_1,x_2)-\frac{e^2}{2^4}\int\int S_{F\mathrm{H}}{}^{e,p}(x_1,y_1)\gamma^\mu\mathfrak{D}_F(y_1-y_2)\,\mathrm{Tr}(\gamma^\mu S_{F\mathrm{HF}}{}^{e,p}(y_2,y_2))S_{F\mathrm{HF}}{}^{e,p}(y_1,x_2)d^4y_1d^4y_2$$

$$-\frac{e^2}{2^4}\int\int S_{F\mathrm{H}}{}^{e,p}(x_1,y_1)\gamma^\mu\mathfrak{D}_F(y_1-y_2)S_{F\mathrm{HF}}{}^{e,p}(y_1,y_2)\gamma_\mu S_{F\mathrm{HF}}{}^{e,p}(y_2,x_2)d^4y_1d^4y_2. \quad (3.1)$$

In terms of Feynman diagrams the Green's function given by Eqs. (3.1) is shown in Fig. 3(a) and the Hartree propagators $-\frac{1}{2}S_{F\mathrm{H}}{}^{e,p}(x_1,x_2)$ are shown in Fig. 3(b).

We see that the propagator $-\frac{1}{2}S_{F\mathrm{H}}{}^{e,p}$ satisfies the equation

$$-\tfrac{1}{2}S_{F\mathrm{H}}{}^{e,p}(x_1,x_2)=-\tfrac{1}{2}S_F(x_1-x_2)$$

$$-\frac{e^2}{2^4}\int\int S_F(x_1-y_1)\gamma^\mu\mathfrak{D}_F(y_1-y_2)$$

$$\times\mathrm{Tr}(\gamma^\mu S_{F\mathrm{H}}{}^{p,e})S_{F\mathrm{H}}{}^{e,p}(y_1,x_2)d^4y_1d^4y_2. \quad (3.2)$$

The last equations for electron and proton constitute the Hartree approximation to the HF equations.

If we apply to Eqs. (3.2) the Dirac operator $(i\gamma^\mu\partial_\mu-m_{e,p})$, we see that the Hartree propagators satisfy the following integrodifferential equations:

$$\left[i\gamma^\mu\partial_\mu+\frac{ie^2}{2^2}\int\mathfrak{D}_F(x_1-y)\gamma^\mu\right.$$

$$\left.\times\mathrm{Tr}(\gamma_\mu S_{F\mathrm{H}}{}^{p,e}(y,y))d^4y-m_{e,p}\right]\left[-\tfrac{1}{2}S_{F\mathrm{H}}{}^{e,p}(x_1,x_2)\right]$$

$$=i\delta^{(4)}(x_1-x_2). \quad (3.3)$$

It is simple to prove that the integral factor which appears in Eqs. (3.3) yields in the nonrelativistic limit and for an infinitely massive proton, the Coulomb interaction between the particles; i.e., Eqs. (3.3), reduce in this limit to the single equation

$$\left(i\gamma^\mu\partial_\mu-\gamma^0\frac{e^2}{4\pi|\mathbf{x}_1|}-m_e\right)\left[-\tfrac{1}{2}S_{F\mathrm{H}}{}^{e}(x_1,x_2)\right]$$

$$=i\delta^{(4)}(x_1-x_2). \quad (3.4)$$

Therefore, the Hartree propagator $-\frac{1}{2}S_{F\mathrm{H}}{}^{e}(x_1,x_2)$ corresponds in the aforementioned approximation to the Green's function of a particle moving in the presence of an external Coulomb field. Hence we can expand the propagators $-\frac{1}{2}S_{F\mathrm{H}}{}^{e,p}(x_1,x_2)$ in terms of a complete set of solutions $\psi_n{}^{e,p}(x)$ of two coupled equations whose Green's functions are the propagators $-\frac{1}{2}S_{F\mathrm{H}}{}^{e,p}(x_1,x_2)$. Thus

$$-\tfrac{1}{2}S_{F\mathrm{H}}{}^{e,p}(x_1,x_2)=\sum_{n,E^+}\psi_n{}^{e,p}(x_1)\bar{\psi}_n{}^{e,p}(x_2)\theta(x_1-x_2)$$

$$-\sum_{n,E^-}\psi_n{}^{e,p}(x_1)\bar{\psi}_n{}^{e,p}(x_2)\theta(x_2-x_1)$$

$$-\psi_{n_0}{}^{e,p}(x_1)\bar{\psi}_{n_0}{}^{e,p}(x_2)\theta(x_2-x_1). \quad (3.5)$$

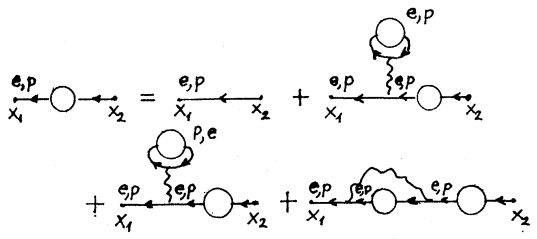

FIG. 2. Relativistic Hartree-Fock equations.

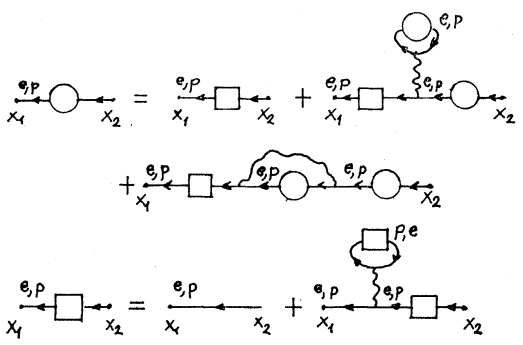

FIG. 3. (a) Hartree-Fock equations. (b) Hartree equations.

The sum over n in the above expression contains also the integration over the continuous spectrum. If the interaction between the particles switched off, Eq. (3.5) must reduce exactly to Eq. (2.3). Therefore, the additional factor n_0 corresponds to our initial state $|p^0q^0\rangle$. But, because we are interested in the bound states of the system, let us consider the other solution of Eq. (3.4) which is given by the same formula (3.5) but now belongs to the discrete part of the spectrum. In this way we introduce explicitly the equations for the bound states from our original equations for scattering states. In the case of two repulsive particles there will be, of course, no bound states and therefore no discrete spectrum.

We can derive now the equations for $\psi^{e,p}(x)$ by projecting on a particular state. We obtain

$$\left[i\gamma^\mu\partial_\mu+\frac{ie^2}{2^2}\int\gamma^\mu\mathfrak{D}_F(x-y)\times\mathrm{Tr}(\gamma_\mu S_{F\mathrm{H}}{}^{p,e}(y^iy))-m_{e,p}\right]\psi_n{}^{e,p}(x)=0. \quad (3.6)$$

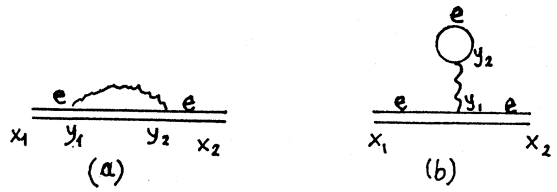

FIG. 4. Second-order radiative corrections to the level shift.

It is straightforward to prove that Eqs. (3.6) correspond to Eqs. (1.3) in the nonrelativistic limit. These equations are the relativistic Hartree approximation to the HF equation (2.10).

We can now prove that the HF equations lead to the ordinary theory with the only difference that our propagators are expressed in terms of the particles which mediate the interaction rather than in terms of external static potentials, that, as we have seen, is an approximation to Eqs. (3.6).

In order to do this let us consider the analog to Eqs. (3.1) when the proton is replaced by a Coulomb field. We have[12]

$$-\tfrac{1}{2}S_F{}^e(x_1,x_2)=-\tfrac{1}{2}S_F{}'^e(x_1,x_2)-\frac{e^2}{2^4}\int S_F{}'^e(x_1,y_1)\gamma^\mu\mathfrak{D}_F(y_1-y_2)S_F{}'^e(y_1,y_2)S_F{}^e(y_2,x_2)d^4y_1d^4y_2$$
$$-\frac{e^2}{2^4}\int S_F{}'^e(x_1,y_1)\gamma^\mu\mathfrak{D}_F(y_1-y_2)\,\mathrm{Tr}(\gamma^\mu S_F{}^e(y_2,y_2))S_F{}^e(y_1,x_2)d^4y_1d^4y_2. \quad (3.7)$$

This equation is equivalent to Eqs. (3.1) except that $-\frac{1}{2}S_F{}^e(x_1,x_2)$ is the Green's function of the following equation:

$$[i\gamma^\mu\partial_\mu-e\gamma^\mu A_\mu{}^{\mathrm{ext}}(x)-m_e]S_F{}'^e(x_1,x_2)=2i\delta^{(4)}(x_1-x_2), \quad (3.8)$$

where $A_\mu{}^{\mathrm{ext}}(x)=(e^2/4\pi|\mathbf{x}|)g_{\mu0}$ and, as we have pointed out, corresponds to Eqs. (3.3) for an infinitely massive proton.

Using now the fact that $\psi_n{}^{e,p}(x)$ are solutions of Eqs. (3.6), we can define an amplitude $f_n{}^{e,p}(x)$ in the following way:

$$f_n{}^{e,p}(x)=-\frac{1}{2}\int_\sigma S_{F\mathrm{HF}}{}^{e,p}(x,x')\gamma^\mu\psi_n{}^{e,p}(x')d\sigma_\mu(x'), \quad (3.9)$$

where σ is any spacelike surface.

Following Schwinger[2] very closely, we obtain, by substituting Eqs. (3.1) for $S_{F\mathrm{HF}}{}^{e,p}$ into (3.9), the following integral equation for $f_n{}^{e,p}(x)$:

$$f_n{}^{e,p}(x)=\psi_n{}^{e,p}(x)+\frac{e^2}{2^3}\int S_{F\mathrm{H}}{}^{e,p}(x,y_1)\gamma^\mu\mathfrak{D}_F(y_1-y_2)S_{F\mathrm{HF}}{}^{e,p}(y_1,y_2)f_n{}^{e,p}(y_2)d^4y_1d^4y_2$$
$$+\frac{e^2}{2^3}\int S_{F\mathrm{H}}{}^{e,p}(x,y_1)\gamma^\mu\mathfrak{D}_F(y_1-y_2)\,\mathrm{Tr}[\gamma^\mu S_{F\mathrm{HF}}{}^{e,p}(y_2,y_2)]f_n{}^{e,p}(y_2)d^4y_1d^4y_2. \quad (3.10)$$

Remembering that $\psi_n{}^{e,p}(x)$ are solutions of Eqs. (3.6), we find that $f_n{}^{e,p}(x)$ satisfy the integrodifferential equations

$$\left(i\gamma^\mu\partial_\mu+\frac{ie^2}{2^2}\int\gamma^\mu\mathfrak{D}_F(x-y)\,\mathrm{Tr}(\gamma^\mu S_{F\mathrm{H}}{}^{p,e}(y,y))d^4y-m_{e,p}\right)f_n{}^{e,p}(x)$$
$$=-\frac{ie^2}{2^2}\int\gamma^\mu\mathfrak{D}_F(x-y)S_{F\mathrm{HF}}{}^{e,p}(x,y)f_n{}^{e,p}(y)d^4y-\frac{ie^2}{2^2}\int\gamma^\mu\mathfrak{D}_F(x-y)\,\mathrm{Tr}(\gamma_\mu S_{F\mathrm{HF}}{}^{e,p}(y,y))f_n{}^{e,p}(y)d^4y. \quad (3.11)$$

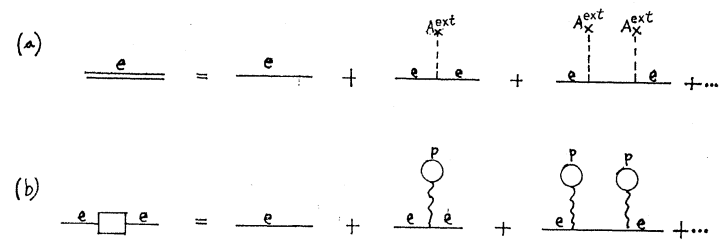

FIG. 5. (a) Electron propagator in the presence of an external field. (b) Electron propagator in the presence of a proton.

Equations (3.11) are the relativistic HF equations which in the Hartree approximation reduce to Eqs. (3.3) and in the nonrelativistic approximation to Eqs. (1.3).

IV. CONCLUSIONS

We now summarize the essential features of the present approach to the relativistic treatment of the two-body problem and the main steps which lead to it.

In the Introduction we showed, by using as an example the nonrelativistic hydrogen atom, that the HF approximation yields the Schrödinger equation in the appropriate limit. We pointed out, therefore, that the HF approximation accounts for the bound states of the system; since the self-consistent field does not contain any initial potential, it corresponds to the Hartree approximation of the HF equations.

The next step consisted in the extension of the HF equations to the relativistic domain. To do this, we generalized the Feynman diagrams which appear in the nonrelativistic HF equations [Fig. 3(a)] and derived the equations that lead to these diagrams (Fig. 2). In order to achieve this goal, we had to express the propagators in terms of one-particle states rather than the vacuum state. Next we showed that the "relativistic HF approximation" is equivalent to the sum of a subset of all the Feynman diagrams which contribute to the interaction between the particles. In second order, all the diagrams are contained in the HF approximation, but in fourth order, for example, the last three of Fig. 1 are excluded.

The last step, Sec. III, was to prove that the HF approximation involves the main part of the interaction, i.e., yields the proper values for the energy shift and linewidth of the bound states. This was achieved very easily by showing that the Hartree approximation, Eq. (3.1), to the relativistic HF equations reduces to the usual theory, Eq. (3.7), in which the proton is replaced by a Coulomb potential, destroying at the same time the covariance of the theory [compare Eqs. (3.6) and (3.8)].

There exists, as is well known, another approach to the relativistic two-body problem, namely, the BS equation. This approach is fully covariant and has proved to be successful in some cases. Nevertheless, it contains some ambiguous features and in its simple version, i.e., the ladder approximation (which as in the HF approximation consists of selecting a subset of Feynman diagrams, namely, ladder diagrams) does not yield in the nonrelativistic limit the motion of a particle in a fixed center of force.[6]

In order to compare our approach with the usual one, let us consider the second-order radiative corrections $\Delta E_\alpha{}^{(2)}$ to the α-level shift. In Fig. 4 we illustrate the corresponding Feynman diagrams. The double lines represent the electron propagator in the external field $A_\mu{}^{\text{ext}}(x)$. The level shift ΔE_α is complex except for the ground state, which is a true stationary state. The real part corresponds to the energy shift and the imaginary part to the linewidth. The infinities which arise from these diagrams must be isolated and canceled against the δm term, which has not been included as explained in Sec. II. The Feynman diagrams of Fig. 4 correspond to second-order terms of Eq. (3.7) and, as pointed out above, the Hartree approximation to the relativistic HF equations is equivalent to Eq. (3.7), except for the fact that the propagator $S_F{}'^e(x_1,x_2)$ satisfies Eq. (3.8) instead of Eq. (3.3). But, as we saw in Sec. III, Eq. (3.3) reduces to Eq. (3.8) if one takes the nonrelativistic limit of the integral factor.

In Fig. 5 we show, in terms of Feynman diagrams, the expansion of $-\frac{1}{2}S_F{}'^e(x_1,x_2)$ of Eq. (3.7) and $-\frac{1}{2}S_{FH}{}^e(x_1,x_2)$ of Eq. (3.1). From Fig. 5(b) we see diagrammatically how the double line is generated as the result of the repeated action of the external field $A^{\text{ext}}(x)$. Figure 5(b) shows explicitly the correspondence between the external field and the proton loops. We stress, though, that the action of the external field does not correspond simply to proton loops. The electron itself contributes to proton loops and more complicated diagrams, like those of Fig. 1, appear in higher orders. In order words and to conclude, we can say that the interaction between the particles arises not through unrealistic external fields, but through a "self-consistent bootstrapping" mechanism, as clearly depicted in the present formulation.

APPENDIX A: NONRELATIVISTIC HF EQUATIONS AND CORRESPONDING FEYNMAN DIAGRAMS

We pointed out in the Introduction that the system of HF equations in the theory of nonrelativistic atoms can be interpreted as a sum of some particular set of Feynman diagrams. We shall discuss here this point in a more explicit form.

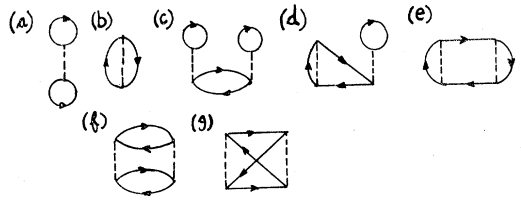

FIG. 6. First- and second-order nonrelativistic Feynman diagrams.

Let us consider the Hamiltonian for many-electron atoms,

$$H=H_0+H_{\text{int}}=-\frac{\hbar^2}{2m}\sum_{(1\leq i\leq N)}\Delta_{\mathbf{r}_i}+\sum_{(1\leq i<j\leq N)}\phi(|\mathbf{r}_i-\mathbf{r}_j|)+\sum_{(1\leq i\leq N)}U(r_i), \quad \text{(A1)}$$

where $U(r_i)=-Ze^2/r_i$ is the single-electron potential energy of the ith electron interacting with the atomic nucleus; $\phi(|\mathbf{r}_i-\mathbf{r}_j|)=e^2/|\mathbf{r}_i-\mathbf{r}_j|$ is the potential energy due to the interaction between the ith and jth electrons; Z is the nuclear charge and N is the total number of electrons.

In second quantization, the Hamiltonian (A1) can be written in the following way:

$$H=\sum_i E_i a_i^\dagger a_i+\tfrac{1}{2}\sum_{ijkl} v_{ij,kl}a_i^\dagger a_j^\dagger a_k a_l, \quad \text{(A2)}$$

where $a_i^\dagger$ and a_i are creation and annihilation operators for electrons in single-electron states $\varphi_i(x)$ which are solutions of the Schrödinger equation for the motion of one electron in the field of the bare nucleus, i.e.,

$$\left[-\frac{\hbar^2}{2m}\Delta_{\mathbf{r}}+U(\mathbf{r})\right]\varphi_i(x)=E_i\varphi_i(x), \quad \text{(A3)}$$

where $x\equiv(\mathbf{r},\sigma)$ and σ is the electron spin.

The matrix elements $v_{ij,kl}$ are given by

$$v_{ij,kl}=\sum_{\sigma,\sigma'}\int d\mathbf{r}\int d\mathbf{r}'\,\varphi_i^*(\mathbf{r},\sigma)\varphi_j^*(\mathbf{r}',\sigma')\phi(|\mathbf{r}-\mathbf{r}'|)\times\varphi_k(\mathbf{r}',\sigma')\varphi_l(\mathbf{r},\sigma). \quad \text{(A4)}$$

Considering for simplicity the case of some nondegenerate atomic state with closed shells which has one electronic state $i\in F$ occupied, and unoccupied ones $i\in G$, we can construct, by using the ordinary Dyson-Wick techniques, the Feynman diagrams which give rise to the correction ΔE of this state, due to the interelectron interaction.

It is necessary to consider only topologically connected diagrams. We obtain in first and second order those diagrams shown in Fig. 6.

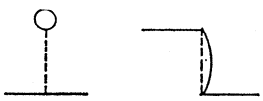

FIG. 7. Self-energy diagrams of first order.

Let us consider now the special set of Feynman diagrams which we call HF diagrams. These correspond to those built up from self-energy parts of first order, i.e., to those shown in Fig. 7. Inserting these diagrams in one of the electronic lines of the first-order diagrams (a) and (b) of Fig. 6, we obtain the HF diagrams of second order. Doing the same thing with the second-order diagrams (c) and (g) of Fig. 6, we obtain the HF diagrams of third order, and so on. The sum of all the diagrams constructed in the way just mentioned is equivalent to the following Green's function:

$$G_{i,i'}^{\text{HF}}(t-t')=G_i^0(t-t')\delta_{ii'}+\frac{i}{\hbar}\int_{-\infty}^{+\infty}dt_1 e^{-\alpha|t_1|}\sum_{kjj'}(v_{j'i,kj}-v_{ji',kj})\times G_i^0(t-t_1)G_{jj'}^{\text{HF}}(-0)G_{ki'}^{\text{HF}}(t_1-t'), \quad \text{(A5)}$$

where

$$G_i^0(t-t')=\langle\Phi_0|\,T(a_i^\dagger(t)a_i(t'))\,|\Phi_0\rangle=e^{-(i/\hbar)E_i(t-t')}[(1-n_i)\theta(t-t')-n_i\theta(t'-t)]$$

$$n_i=\begin{cases}1, & i\in F\\ 0, & i\in G\end{cases} \quad \text{(A6)}$$

is the electron propagator in the absence of the other electrons, i.e., the single electron propagator affected only by the atomic nucleus.

The energy shift ΔE is given by

$$\Delta E_{\text{HF}}=\frac{1}{2}\int_0^1\frac{dg}{g}\sum_j\left(\frac{\hbar}{i}\frac{\partial}{\partial t}+E_j\right)\times G_{j,j}^{\text{HF}}(t;t+0|g)\Big|_{t=0}, \quad \text{(A7)}$$

where g is the intensity parameter for the interaction between the electrons and appears in $H=H+gH_{\text{int}}$.

The diagrammatic representation of Eq. (A6) is shown in Fig. 8.

Solving Eq. (A6) graphically, it is quite easy to see that it contains in fact all the diagrams which we have called HF diagrams.

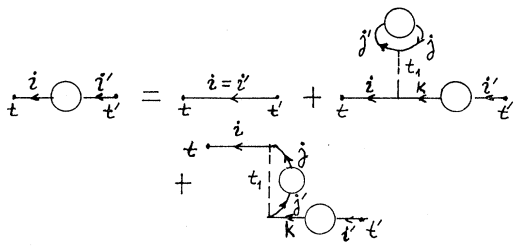

FIG. 8. Nonrelativistic Hartree-Fock equations.

It is simple to prove now that the HF Green's function (A6) has the form

$$G_{ii'}{}^{\mathrm{HF}}(t-t')=\sum_s C_{is}C_{i's}^* \times e^{-(i/\hbar)\epsilon_s(t-t')}[(1-\nu_s)\theta(t-t')-\nu_s\theta(t'-t)], \quad \text{(A8)}$$

where $\nu_s=n_s$, and C_{is} obey the well-known HF equations or

$$(E_i-\epsilon_p)C_{ip}+\sum_{kjj'}(v_{j'i,kj}-v_{ij',kj}) \times(\sum_s C_{js}C_{j's}^*\nu_s)C_{kp}=0, \quad \text{(A9)}$$

which, as is well known, were originally derived from a variational principle.

APPENDIX B: GENERALIZATION OF WICK THEOREM

Wick's theorem relates the T-product of field operators with the sum of N-products of the same operators with all possible sets of contractions.[21] We have

$$T\{\chi(x_1)\cdots\chi(x_n)\}=\sum_{\text{contractions}} N\{\chi(x_1)\cdots\chi(x_n)\}, \quad \text{(B1)}$$

where the sum is over all sets of contractions. The χ's refer to electron-positron field operators. By definition, the T-product orders the operators according to their time arguments, and the N-product orders them in such a way that all annihilation operators stand to the right of creation operators. For $n=2$, the contractions defined in relation (B1) are given by

$$T\{\chi(x_1)\chi(x_2)\}=N\{\chi(x_1)\chi(x_2)\}+\chi\cdot(x_1)\chi\cdot(x_2), \quad \text{(B2)}$$

where $\chi\cdot(x_1)\chi\cdot(x_2)$ represents the contracted factors.

According to the usual separation of the fields into positive- and negative-frequency parts [see Eq. (2.6′)], we have, on account of the fact that $\psi^{(+)}(x)|0\rangle=\bar{\psi}^{(+)}(x)|0\rangle=0$,

$$\langle 0|N\{\chi(x_1)\cdots\chi(x_n)\}|0\rangle=0, \quad \text{(B3)}$$

where

$$\psi^{(+)}(x)=\frac{1}{(2\pi)^{3/2}}\int_{p_0>0} d^3p \times\left(\frac{m}{E(\mathbf{p})}\right)^{1/2}\sum_{r=1}^{2} b_r(\mathbf{p})\omega^r(\mathbf{p})e^{-ip\cdot x},$$

$$\psi^{(-)}(x)=\frac{1}{(2\pi)^{3/2}}\int_{p_0>0} d^3p \times\left(\frac{m}{E(\mathbf{p})}\right)^{1/2}\sum_{r=1}^{2} d_r^{\dagger}(\mathbf{p})v^r(\mathbf{p})e^{ip\cdot x}, \quad \text{(B4)}$$

and $\bar{\psi}(x)=\psi^{\dagger}(x)\gamma^0$.

The generalized Wick theorem[22] is quite analogous to the ordinary one, with the only difference that instead of considering the vacuum state $|0\rangle$, we consider now the one-electron state $|q_0{}^{r_0}\rangle=b_{r_0}{}^{\dagger}(\mathbf{q}_0)|0\rangle$. In order to apply Wick's theorem for this state rather than the vacuum state, we must redefine the N-product. (We point out here that in order to prove Wick's theorem, we make use of the fact that we have two different ways of ordering the operators and not the specific properties of the T- and N-products, as will be clear later on.) To redefine the N-product, we perform a somewhat different separation of the field operators, namely,

$$\psi^{(+)}(x)=\frac{1}{(2\pi)^{3/2}}\int_{p_0>0;\ p\neq q_0{}^{r_0}} d^3p \times\left(\frac{m}{E(\mathbf{p})}\right)^{1/2}\sum_{r=1}^{2} b_r(\mathbf{p})\omega^r e^{-ip\cdot x},$$

$$\psi^{(-)}(x)=\frac{1}{(2\pi)^{3/2}}\int_{p_0>0} d^3p\left(\frac{m}{E(\mathbf{p})}\right)^{1/2}\sum_{r=1}^{2} d_r^{\dagger}(\mathbf{p})v^r e^{ip\cdot x} +\frac{1}{(2\pi)^{3/2}}\left(\frac{m}{E(\mathbf{q}_0)}\right)^{1/2} b_{r_0}(\mathbf{q}_0)\omega^r(\mathbf{q}_0)e^{-ip\cdot x}. \quad \text{(B5)}$$

The new N-product will order the field operators in such a way that the new $\psi^{(-)}(x)$ operators will stand to the right of the new operators defined by relations (B5). Because of this new separation, we now have

$$\psi^{(+)}(x)|q_0{}^{r_0}\rangle=\bar{\psi}^{(+)}(x)|q_0{}^{r_0}\rangle=0,$$

and consequently

$$\langle q_0{}^{r_0}|N[\chi(x_1)\cdots\chi(x_n)]|q_0{}^{r_0}\rangle=0. \quad \text{(B6)}$$

With this new definition of the N-product, the generalized Wick theorem can be proved in a way similar to the ordinary one, by using mathematical induction.[22]

[22] V. Tolmachev, Advan. Chem. Phys. 14, 421 (1969).