Time-dependent functional theory of coupled electron and electromagnetic fields in condensed-matter systems

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It is shown that a time-dependent external four-vector potential $a_\mu^{\rm ext}(\vec{r}t)$ and a conserved external four-current $j_\mu^{\rm ext}(\vec{r}t)$, with a given fixed initial state of the combined condensed-matter–electromagnetic system, lead, respectively, to a conserved self-consistent four-current density $J_\mu(\vec{r}t)$ and a self-consistent four-vector field $A_\mu(\vec{r}t)$, such that a map $(a_\mu^{\rm ext}, j_\mu^{\rm ext})\rightarrow(J_\mu, A_\mu)$ is invertible under certain simple conditions. With this as a basis, the stationary action principle is used to derive the self-consistent equations for the electron and the electromagnetic fields appropriate for a description of the combined condensed-matter and electrodynamic systems, where real or virtual pair creation is ignored.

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I. INTRODUCTION

Density-functional theory for stationary states or ensembles is a formulation of many-body theory. It is now a mature subject with many successful applications. For a review of this, one may consult the book by Dreizler and Gross [1]. A general formulation covering essentially all time-dependent potentials was given ten years ago by Runge and Gross [2]. A review of this subject covering subsequent work is found in an article by Gross and Kohn [3]. This theory is not as fully implemented to the same extent as the stationary state theory, but it is a powerful method for attacking a much wider class of many-body problems of interacting electrons of condensed matter. This is because the important many-body effects of correlations and interactions are all incorporated into a functional, which in turn determines, in principle, the electronic properties of the system under consideration. In almost all condensed-matter problems, except those with high atomic number ($Z \geq 50$) elements, a nonrelativistic description of the electrons suffices. However quantum electrodynamics (QED) furnishes a fundamental basis on which quantum theory of a system of interacting electrons can be based. This is because the formalism of QED is particularly convenient since all the interaction between a charged particle and an electromagnetic field, which must be expressed in a relatively cumbersome manner in ordinary nonrelativistic quantum mechanics, is contained in a single simple term. A time-independent functional theory based on this formalism is given by Rajagopal and Callaway [4]. These authors were not significantly concerned with relativistic effects and proceeded to the nonrelativistic limit after the general principles were described. Their aim was to incorporate electronic systems with magnetic order, such as ferromagnetic or spin-density-wave states. This theory has also been employed to examine other problems where magnetic interactions are of importance [5], such as magnetic anisotropy, nuclear magnetic shielding, etc. A time-dependent functional formalism for many-electron systems subjected to external electromagnetic fields with arbitrary time dependence *but treated as classical fields,* is given by Ghosh and Dhara [6], thus extending the work of Runge and Gross [2] to time-dependent vector potentials.

In order to include a description of the physics and chemistry of condensed-matter systems composed of heavy elements ($Z \geq 50$), the relativistic effects need to be incorporated and a functional theory was developed by the author and his co-workers [7]. This work may be considered as a functional formulation of the relativistic many-body problem of quantum plasma and radiation [8,9]. This theory encounters serious self-interaction problems and the use of the renormalization program of Feynman-Schwinger formulation of QED provides results in which all observable quantities are finite. In the functional context, Engel [10] has described the changes needed for the stationary, time-independent external fields. The end result is that one works with renormalized quantities. It should be remarked that the full numerical implementation of the relativistic functional theory is not at hand at present, but holds promise for the future.

It may not be out of place here to remark that a fully field-theoretical treatment of the time-dependent fields involves further difficulties when the field strengths are strong enough to produce electron-positron pairs [11]. A phase-space approach has recently been investigated [12], and a method of adiabatic regularization combined with mean-field approximation for a homogeneous time-dependent electric field has been examined [13]. As will be described below, in the problems of condensed-matter systems we are considering, we do not anticipate such problems and thus the functional formulation we offer here comes with this caveat.

The purpose of this paper is to set up a time-dependent (td) functional theory of coupled condensed matter (M) and electromagnetic (em) fields are not considered hitherto, which will provide a formal framework *to study both the matter and electromagnetic equations on the same*

footing. Such a nonperturbative theory is required when the interaction between the fields and the matter system is strong. Several examples of this are the electrodynamics of superconductors, laser interactions with matter, charge-carrier behavior in very high frequency nanoelectronic devices, etc. In these condensed-matter problems a nonrelativistic description of the matter field suffices. However, a relativistic description of the matter field is often used as in our earlier work [4,7], because it lends an elegant description of the system including a wide variety of the magnetic properties of condensed matter [5]. As we do not envisage electron-positron pair production in our systems, we will not formulate the theory to include this here. The fully self-consistent approach proposed here is expected to bring out novel, highly nonlinear phenomena in these systems, which are traditionally handled non-self-consistently using phenomenological (e.g., mean-field) procedures. In the past only the equation for the electron in the absence of the quantized electromagnetic fields was formulated in the functional framework in the presence of external classical (unquantized) scalar and vector potentials so as to take into account the interactions among the particles [6]. For a discussion of such an approach one may refer to the book by Dreizler and Gross [6]. Recently, Kohn, Gross, and Oliveira [14] developed a functional theory of the electron system of a superconductor in a magnetic field treating the electromagnetic fields classically, but they were put in an *ad hoc* self-consistency loop for the vector potential. A more complete theory would obtain the two equations within a single framework, and it is this feature that is addressed here. In order to keep our development pertinent to condensed-matter systems, here we develop a theory that yields the equations for matter and electromagnetic fields applicable under a wide variety of situations of the types mentioned above. By doing this it will also become clear as to when these two equations can be discussed separately, as has often been done in the past [4,7].

The basic idea is to recognize that we have here an interacting pair of quantum fields with the matter four-current density coupled to the external electromagnetic sources, while the internal electromagnetic fields are coupled to the external four-current density. This was traditionally studied in the past by perturbative diagrammatic techniques, without invoking full self-consistency. As mentioned above, the functional theory exists only for the matter field while either ignoring or treating the other field classically. Here we fill this gap and develop the time-dependent functional theory in the same spirit as was done for the other important pair of interacting fields of importance in condensed-matter physics, namely the electron-ion system [15], based on the earlier work of Runge and Gross [2] for td-pure states. For a review of this pure-state td-functional theory, see Ref. [3].

In Sec. II, we give a brief description of the system under consideration along with the various points mentioned above concerning renormalization, pair production, etc. In Sec. III, the basic theorems of our functional theory are stated and proved. In Sec. IV, some proposed applications of the theory are given. In the final Sec. V, future plans and concluding remarks are given.

II. DESCRIPTION OF THE SYSTEM

The time evolution of the coupled matter-electrodynamic system along with their interactions with external sources is governed by the equation [11] for the state vector of the system:

$$\left| i\hbar\frac{\partial}{\partial t}-\hat{H}(t)\right| |\Psi(t)\rangle=0\ ,\quad \text{given } |\Psi(t_0)\rangle\ , \tag{1}$$

where $\hat{H}$ in the Schrödinger representation is

$$\hat{H}=\hat{H}_M+\hat{H}_E+\hat{H}_{\rm int}+\hat{H}_{\rm ext}+E_{\rm vac}\ . \tag{2}$$

$E_{\rm vac}$ is the vacuum expectation value of $\hat{H}$ is in Ref. [11], which we ignore in the subsequent development without loss of clarity. Here we use the Dirac field to represent the matter Hamiltonian to keep the discussion in some generality (but with a caveat mentioned above), so as to include discussion of magnetic properties of the system as well, in the same spirit as the work done by the author and his co-workers [4,7] and others [5]. All the operators are in Heisenberg representation.

$$\hat{H}_M(\hat{\bar{\psi}},\hat{\psi})=\int d^3r :\hat{\bar{\psi}}(\vec{r}t)(-i\hbar\vec{\gamma}\cdot\vec{\nabla}+m_0c^2)\hat{\psi}(\vec{r}t): \tag{2a}$$

the electromagnetic part is

$$\hat{H}_E(\partial_\mu\hat{A}^\nu)=\tfrac{1}{2}\int d^2r :(\hat{\vec{E}}^2+\hat{\vec{B}}^2): ,$$
$$\hat{\vec{E}}=-\frac{1}{c}\frac{\partial\hat{\vec{A}}}{\partial t}-\vec{\nabla}\hat{A}_0,\hat{\vec{B}}=(\vec{\nabla}\times\hat{\vec{A}})\ , \tag{2b}$$

the matter-electromagnetic interaction is

$$\hat{H}_{\rm int}=\int d^3r :\hat{j}_\mu(\vec{r}t)\hat{a}^\mu(\vec{r}t): \tag{2c}$$

and the interaction of both of these with explicitly td external sources is given by

$$\hat{H}_{\rm ext}=\int d^3r :[\hat{j}_\mu(\vec{r}t)a^\mu_{\rm ext}(\vec{r}t)+j^{\rm ext}_\mu(\vec{r}t)\hat{A}^\mu(\vec{r}t)]: . \tag{2d}$$

Here: : stands for normal ordering of operators. The route to the Hamiltonian from the Lagrangian may be found in Ref. [11]. The notations used here are different from those in Ref. [4], since we employ the normal ordering of operators and separate out the $E_{\rm vac}$ term in Eq. (2), and the relationship of the two may be found in Ref. [11]. We have chosen Eq. (2d) in a somewhat unconventional symbolic form for specifying the external sources $a^{\rm ext}_\mu$ *and* $j^{\rm ext}_\mu$, for two reasons: (1) we have in mind different classes of physical problems requiring specification of one or the other; and (2) $j^{\rm ext}_\mu$ is traditionally used in the formal theoretical framework of field theory to generate the various interaction contributions. In particular, $a^{\rm ext}_\mu$ is specified in some external magnetic-field problems which couples to the M current, and $j^{\rm ext}_\mu$ is specified in radiation source problems which couple to the em field. Conventionally we would attack these two problems separately, and the development of the functional formalism presented would proceed as given here in these two cases. From a field-theoretical point of view, $j^{\rm ext}_\mu$ is traditionally useful as a source term to generate the necessary quantum elec-

trodynamic contributions in dealing with coupled M and em fields. As we shall see toward the end of this paper (Theorem 3) this choice leads to an elegant, symmetric form for the ensuing self-consistent equations of motion for the M and em fields in our functional formalism. We specify the external four-potential in the Lorentz gauge

$$\partial_\mu a^\mu_{\text{ext}}(\vec{r}t)=0 , \tag{3}$$

and the Fermion four-current operator in the Schrödinger representation is

$$\hat{j}_\mu(\vec{r})=:\hat{\bar{\psi}}(\vec{r})\gamma_\mu\hat{\psi}(\vec{r}): , \tag{4}$$

which obeys the continuity equation in the Heisenberg picture [denoted by subscript H; all the operators in Eq. (2) and in later discussions are in the Heisenberg representation where we do not indicate by subscript H]

$$\partial_\mu \hat{j}^\mu_H=0 , \tag{5}$$

as does the external source current

$$\partial_\mu j^\mu_{\text{ext}}(\vec{r}t)=0 . \tag{6}$$

These conditions assure us of the gauge covariance of the theory. The Fermion field operator for matter $\hat{\bar{\psi}}$ and $\hat{\psi}$ and the electromagnetic field operators $\hat{A}_\mu$ and their canonical conjugates obey standard commutation relations at equal times among themselves [4] in a chosen gauge. We also choose the Lorentz gauge for the em field for the present in order to keep the discussion relativistically covariant. The choice of the Lorentz gauge maintains the formal framework explicitly relativistically covariant, even though it poses some technical problems requiring certain procedures which do not invalidate our development here. In actual computations in condensed-matter problems, the standard choice of gauge is the Coulomb gauge, which has certain advantages at the expense of a loss of covariance, but one maintains gauge covariance by appropriate standard manipulations [11]. For more details of these aspects of the em-field theory, one may refer to recent textbooks [11,16,17(a),17(b)]. The gauge covariance and representations of the fields are discussed in detail by Engel [10]. The expressions given above are gauge covariant in the usual sense. However, there is another place where the question of the gauge comes up again when we consider the mapping theorem, Theorem 1, to be discussed presently. Following Engel [10] we may state here that a class of four potentials differing by a gauge transformation lead to the same four currents so that no contradictions occur. This was pointed out by the present author in developing the relativistic functional theory [4]. We will address questions of renormalizations in some detail; those for the time-independent case are discussed by Engel [10]. The divergent vacuum energies are eliminated by normal ordering of operators. The ultraviolet divergences of the quantized em field are eliminated by the standard method of absorbing them in a redefinition of coupling constants. In the work of Engel, it is shown that the result of renormalization in the functional theory leads to counter terms which are universal functionals of external potential and renormalized current. Following Ref. [11], we recall that there is no analog for the vacuum state in the presence of time-dependent fields. But if $\hat{A}_\mu(\vec{r}t)$ is constant for both remote past and future times, then these two vacuum states in these two regions can be defined separately, so that the overlap of these two states describes the probability amplitude of the persistence of the vacuum state. Also the vacuum state is defined by specifying which of the single-particle states are empty and which are filled, with the filled states being interpreted as antiparticles and the unfilled states as particles. We start by defining a Fermi energy and the set of "occupied" states as those whose energies are below the Fermi energy. This vacuum becomes charged, and reduces its energy by emitting electron-positron pairs for energies of the order of $2mc^2$, which is of order 1 Mev. As estimated in Ref. [11], superstrong fields are needed to produce such effects, and we certainly do not encounter such large energies with the types of fields employed in condensed-matter laser experiments. Thus we are outside the realm of pair production possibilities in our framework. With this caveat, the standard renormalization techniques leave these features intact in the time-dependent theory proposed here.

The time-dependent equation for the state vector for the coupled system in the Schrödinger representation Eq. (1) can be deduced from the stationary property of the action functional:

$$A(t_0,t_1)=\int_{t_0}^{t_1}dt\left\langle\Psi(t)\left|\left[i\hbar\frac{\partial}{\partial t}-\hat{H}(t)\right]\right|\Psi(t)\right\rangle . \tag{7}$$

The four-potential and four-current operators possess the expectation values

$$J_\mu(\vec{r}t)=\langle\Psi(t)|\hat{j}_\mu(\vec{r})|\Psi(t)\rangle , \tag{8}$$

$$A_\mu(\vec{r}t)=\langle\Psi(t)|\hat{A}_\mu(\vec{r}t)|\Psi(t)\rangle . \tag{9}$$

The expectation value defined in Eq. (9) may be thought of as arising from the use of a "coherent state" representation [18], or as some other suitable superposition of number states for the vector $|\Psi(t)\rangle$. We now state and prove the mapping theorem in Sec. III.

III. BASIC THEOREMS OF THE FUNCTIONAL THEORY

Theorem 1. If processes involving real or virtual pair creation are neglected, then for every $(a^{\text{ext}}_\mu, j^{\text{ext}}_\mu)$ which can be expanded into respective Taylor series in the time coordinate around the initial time t_0, a map which preserves the continuity Eqs. (5) and (6),

$$(a^{\text{ext}}_\mu, j^{\text{ext}}_\mu)\rightarrow(J_\mu, A_\mu) \tag{10}$$

is defined by solving the td equation (1) for the state vector of the combined system in the Schrödinger representation, with a fixed initial state $|\Psi(t=t_0)\rangle=|\Psi_0\rangle$, and calculating the corresponding quantities $J_\mu(\vec{r}t)$ and $A_\mu(\vec{r}t)$ given by using Eqs. (8) and (9). This map is invertible under certain simple conditions.

Proof. We consider those states which evolve from a fixed given initial state $|\Psi_0\rangle$. The time evolution of an ar-

bitrary operator $\hat{O}(t)$, which may in general be explicitly time dependent, is given by

$$i\hbar\frac{d}{dt}\langle\Psi(t)|\hat{O}(t)|\Psi(t)\rangle = \langle\Psi(t)|i\hbar\frac{\partial}{\partial t}\hat{O}(t)+[\hat{O}(t),\hat{H}(t)]_-|\Psi(t)\rangle \ . \quad (11)$$

We need to show that (J_μ, A_μ) and (J'_μ, A'_μ) corresponding to $(a_\mu^{\rm ext}, j_\mu^{\rm ext})$ and $(a_\mu^{\prime\rm ext}, j_\mu^{\prime\rm ext})$ are different under certain conditions. Remembering that we consider only those states that evolve from a fixed initial state $|\Psi_0\rangle$, we have

$$\begin{aligned} i\hbar\frac{d}{dt}[J_\mu(\vec{r}t)-J'_\mu(\vec{r}t)]_{t=t_0} &= \langle\Psi_0|[\hat{j}_\mu(\vec{r}t_0),\hat{H}(t_0)-\hat{H}'(t_0)]_-|\Psi_0\rangle \\ &= \int d^3r_1\langle\Psi_0|[\hat{j}_\mu(\vec{r}t_0),\hat{j}_{\mu_1}(\vec{r}_1t_0)]_-|\Psi_0\rangle \\ &\quad\times[a_{\rm ext}^{\mu_1}(\vec{r}_1t_0)-a_{\rm exp}^{\prime\mu_1}(\vec{r}_1t_0)] \ , \end{aligned} \quad (12a)$$

$$\left|i\hbar\frac{d}{dt}\right|^2[J_\mu(\vec{r}t)-J'_\mu(\vec{r}t)]_{t=t_0} = i\hbar\int d^3r_1\langle\Psi_0|[\hat{j}_\mu(\vec{r}t_0),\hat{j}_{\mu_1}(\vec{r}_1t_0)]_-|\Psi_0\rangle \times\left|\frac{d}{dt}\right|(a_{\rm ext}^{\mu_1}(\vec{r}_1t)-a_{\rm ext}^{\prime\mu_1}(\vec{r}_1t))_{t=t_0} \ , \quad (12b)$$

and, similarly, higher-order time derivatives are obtained. The commutator appearing in Eqs. (12a) and (12b) is evaluated by using the equal time commutation rule for Dirac fields:

$$[\hat{j}_\mu(\vec{r}t_0),\hat{j}_{\mu_1}(\vec{r}_1t_0)]_- = \delta(\vec{r}-\vec{r}_1):\hat{\bar{\psi}}(\vec{r}t_0)[\gamma_\mu,\gamma_{\mu_1}]_-\hat{\psi}(\vec{r}t_0): \ , \quad (12c)$$

and its expectation value appearing there is, in general, nonzero. And

$$i\hbar\frac{d}{dt}[A_\mu(\vec{r}t)-A'_\mu(\vec{r}t)]_{t=t_0} = \langle\Psi_0|[\hat{A}_\mu(\vec{r}t_0),\hat{H}(t_0)-\hat{H}'(t_0)]_-|\Psi_0\rangle = \int d^3r_1[j_{\mu_1}^{\rm ext}(\vec{r}_1t_0)-j_{\mu_1}^{\rm ext}(\vec{r}_1t_0)]\langle\Psi_0|[\hat{A}_\mu(\vec{r}t_0),\hat{A}^{\mu_1}(\vec{r}_1t_0)]_-|\Psi_0\rangle = 0 \ , \quad (13a)$$

$$\left|i\hbar\frac{d}{dt}\right|^2[A_\mu(\vec{r}t)-A'_\mu(\vec{r}t)]_{t=t_0} = 0 \ , \quad (13b)$$

$$\left|i\hbar\frac{d}{dt}\right|^3[A_\mu(\vec{r}t)-A'_\mu(\vec{r}t)]_{t=t_0} = (i\hbar)^2\left|\frac{d}{dt}\right|[j_{\mu_1}^{\rm ext}(\vec{r}t)-j_{\mu_1}^{\prime\rm ext}(\vec{r}t)]_{t=t_0}g_\mu^{\mu_1} \ . \quad (13c)$$

In Eq. (13a) we obtain zero because of the Lorentz gauge commutation rules for the vector field operators [17a] as well as due to the initial condition on the currents. In Eq. (13b), we obtain two terms, each of which is zero, one due to the initial conditions and the other due to the commutation rules for the vector fields. Equation (13c) shows that the first nonzero derivative is of third order, and subsequent higher-order time derivatives involve corresponding higher-order time derivatives on the right-hand side. Here $g_\mu^{\mu_1}$ is the standard metric tensor [10]. Thus, knowing the commutation rules, it is clear that (J_μ, A_μ) and (J'_μ, A'_μ) will become different at infinitesimally later times than t_0. The simple conditions mentioned above are thus the nonzero values for the time derivatives of $a_\mu^{\rm ext}, j_\mu^{\rm ext}$ as required in Ref. [2]. The nonrelativistic counterpart for the M field in the presence of $a_\mu^{\rm ext}(\vec{r}t)$ with *em field treated as a classical c-number field* is given in a paper by Ghosh and Dhara [6]. It should be pointed out that the M field in the Dirac formulation given here is simpler in its formal structure than its nonrelativistic counterpart, because the four-current operator in this framework does not depend explicitly on the em fields. Of course, a Gordon decomposition exposes the physical content of the current operators (see Ref. [4] for the Gordon decomposition of the four-current operator), Eq. (4), but is not essential for the present argument. We will now go on to develop further the functional theory in much the same way as in Refs. [2] and [15].

We have thus proved the central result of the theory that

$$|\Psi(t)\rangle = |\Psi[J_\mu(\vec{r}t), A_\mu(\vec{r}t)]\rangle$$

and the expectation value of any arbitrary operator is also a functional of J_μ, A_μ:

$$\langle\Psi(t)|\hat{O}|\Psi(t)\rangle = O[J_\mu(\vec{r}t), A_\mu(\vec{r}t)] \ .$$

Theorem 2. The stationary property of the action, Eq. (7), leads to the td equation (1) for the state vector for the combined system in the Schrödinger representation. This functional may now be written as a functional of J_μ, A_μ in view of Theorem 1:

$$\mathcal{A}[J_\mu, A_\mu] = \mathcal{B}[J_\mu, A_\mu] - \int_{t_0}^{t_1}dt\int d^3r[J_\mu(\vec{r}t)a_{\rm ext}^\mu(\vec{r}t) + j_\mu^{\rm ext}(\vec{r}t)A^\mu(\vec{r}t)] \ , \quad (14)$$

where $\mathcal{B}[J_\mu, A_\mu]$ is a universal functional of the td-current densities and the td fields for a given fixed initial

state. $\mathcal{A}[J_\mu, A_\mu]$ is stationary at exact J_μ, A_μ of the given system, and can be computed from the Euler equations

$$\frac{\delta\mathcal{A}[J_\mu, A_\mu]}{\delta J_\mu}=0 \quad \text{and} \quad \frac{\delta\mathcal{A}[_\mu, A_\mu]}{\delta A_\mu}=0 \ . \tag{15}$$

As in Theorem I, processes involving real or virtual pair creation are neglected here.

Proof. Equation (14) follows directly from the definitions, Eq. (2), and the constructions, Eqs. (8,9). In fact we have

$$\mathcal{B}[J_\mu, A_\mu]=\int_{t_0}^{t_1} dt \langle \Psi[J_\mu(\vec{r}t), A_\mu(\vec{r}t)]| \times \left[i\hbar\frac{\partial}{\partial t}-\hat{H}_M-\hat{H}_E-\hat{H}_{\text{int}} \right] \times |\Psi[J_\mu(\vec{r}t), A_\mu(\vec{r}t)]\rangle \ . \tag{16}$$

Since the action Eq. (7) is stationary for the exact solution of the td equation, the corresponding functional must also be stationary for the exact td currents and fields.

In order to derive practical systems of equations, we need to employ a suitable state vector $|\Psi[J_\mu(\vec{r}t), A_\mu(\vec{r}t)]\rangle$. For example, one way to obtain the familiar equations is to employ a product of state vectors pertaining to the M and em systems, with the em system being either a coherent state as mentioned earlier or a superposition of number states, each separately normalized to unity as a possible approximation, which is valid for noninteracting systems. This then allows us to examine the coupling of em and M systems within a self-consistent functional scheme. Then the functional $\mathcal{B}$ in Eq. (16) takes the form

$$\mathcal{B}[J_\mu, A_\mu]\cong\mathcal{B}_M[J_\mu]+\mathcal{B}_E[A_\mu]+\mathcal{B}_{\text{int}}[J_\mu, A_\mu] \ . \tag{17}$$

Here

$$\mathcal{B}_M[J_\mu]=\int_{t_0}^{t_1} dt \langle \Psi_M[J_\mu(\vec{r}t)]| \times \left[i\hbar\frac{\partial}{\partial t}-\hat{H}_M \right] |\Psi_M[J_\mu(\vec{r}t)]\rangle \ , \tag{18a}$$

$$\mathcal{B}_E[A_\mu]=\int_{t_0}^{t_1} dt \langle \Psi_E[A_\mu(\vec{r}t)]| \times \left[i\hbar\frac{\partial}{\partial t}-\hat{H}_E \right] |\Psi_E[A_\mu(\vec{r}t)]\rangle \ , \tag{18b}$$

and

$$\mathcal{B}_{\text{int}}[J_\mu, A_\mu]=\int_{t_0}^{t_1} dt \langle \Psi_M|\langle \Psi_E| \times \int d^3r :\hat{j}_\mu(\vec{r})\hat{A}^\mu(\vec{r}):|\Psi_E\rangle|\Psi_M\rangle \ . \tag{18c}$$

From this we derive the familiar equations for the electrons and electrodynamic fields. Further research into the use of possible state vectors is called for to go beyond this familiar scheme. Here we state another theorem whose proof follows in a straightforward way, which is a set of coupled matter and electromagnetic field equations in the functional formalism.

Theorem 3. The effective Dirac and Maxwell equations of the functional theory are

$$i\hbar\frac{\partial}{\partial t}\phi_i(\vec{r}t)=\left\{ \vec{\alpha}\cdot\left[-i\hbar\vec{\nabla}-\frac{e}{c}\vec{A}_{\text{eff}}(\vec{r}t) \right] +m_0(1-\beta)+A_{\text{eff}0}(\vec{r}t) \right\}\phi_i(\vec{r}t) \ , \tag{19}$$

where

$$J_\mu(\vec{r}t)=\sum_i \text{tr}[\phi_i^*(\vec{r}t)\alpha_\mu\phi_i(\vec{r}t)] \ , \tag{19a}$$

$$A_{\text{eff}\mu}(\vec{r}t)=a_{\text{ext}\mu}(\vec{r}t)+A_\mu(\vec{r}t)+\frac{\delta\tilde{\mathcal{B}}[J^\mu, A^\mu]}{\delta J_\mu(\vec{r}t)} \ , \tag{19b}$$

$$\tilde{\mathcal{B}}[J_\mu, A_\mu]=\mathcal{B}_M^s[J_\mu]+\mathcal{B}_E^s[A_\mu] +\int_{t_0}^{t_1} dt \int d^3r \, J^\mu(\vec{r}t)A_\mu(\vec{r}t) -\mathcal{B}[J_\mu, A_\mu] \ , \tag{19c}$$

with

$$\mathcal{B}_M^s[J_\mu]=\int_{t_0}^{t_1} dt \langle \Phi_M^s[J_\mu(\vec{r}t)]| \times \left[i\hbar\frac{\partial}{\partial t}-\hat{H}_M \right] |\Phi_M^s[J_\mu(\vec{r}t)]\rangle \ , \tag{19d}$$

$$\mathcal{B}_E^s[A_\mu]=\int_{t_0}^{t_1} dt \langle \Phi_E^s[A_\mu(\vec{r}t)]| \times \left[i\hbar\frac{\partial}{\partial t}-\hat{H}_E \right] |\Phi_E^s[A_\mu(\vec{r}t)]\rangle \ , \tag{19e}$$

and

$$\partial_m F^{\mu\nu}=\partial_\mu[\partial^\mu A^\nu(\vec{r}t)-\partial^\nu A^\mu(\vec{r}t)]=J_{\text{eff}}^\nu(\vec{r}t) \ , \tag{20}$$

where

$$J_{\text{eff}}^\nu(\vec{r}t)=j_{\text{ext}}^\nu(\vec{r}t)+J^\nu(\vec{r}t)+\frac{\delta\tilde{\mathcal{B}}[J^\mu, A^\mu]}{\delta A^\nu} \ . \tag{21}$$

In Eq. (21), $J_\mu(\vec{r}t)$ is the same as in Eq. (19a). As in the previous theorems, processes involving real or virtual pair creation are neglected here. As before, the functional $\tilde{\mathcal{B}}[J^\mu, A^\mu]$ depends on the given initial state, and represents important contributions due to all the interactions and correlations in the system.

The usual Hartree-like term [3] is not explicitly shown here in part because it arises naturally when a Coulomb gauge is used for the em field. The separations shown in Eqs. (19c)–(19e) are not unique but are made so as to retain the appearance of the usual field equations [16]. We may also point out that the "noninteracting" actions $\mathcal{B}_M^s$ and $\mathcal{B}_E^s$ are chosen so as to give, respectively, the same $J_\mu(\vec{r}t)$ and $A_\mu(\vec{r}t)$ as for the interacting problem, as is usually done in the functional formalism [3].

Equations (19) and (20) are now coupled matter and electromagnetic field equations. These could be recast in different forms by rewriting $\mathcal{B}$ in such a way as to

separate the familiar structures (e.g., Hartree term) from them, and writing the remainder as the correlated part contributions. As a way of handling renormalization effects, we may rewrite the above equations in terms of the traditional Green functions for the electron and the electromagnetic fields.

IV. PROPOSED APPLICATIONS

The above development was designed to address the evolution of a pure state, given the specification of the given initial conditions as above in the Schrödinger representation. A much larger class of problems need a more general setting involving nonequilibrium statistical mechanics involving the matrix Green-function approach using the system density matrix when one considers a system which is initially given to be in thermal equilibrium and is subjected to external td forces of the types considered above. In the context of nonrelativistic quantum plasmas and quantized radiation, such a field-theoretical approach was given some time ago by DuBois [8]. Bezzerides and DuBois [9] generalize the theory given in Ref. [8] to Dirac electrons so as to treat the quantum electrodynamics of ultrarelativistic quantum plasmas. As stated in Sec. I, there are many other contexts in which such a formulation is required *even if we are not in the ultrarelativistic limit,* and the motivation of the present work is to develop a self-consistent method which goes beyond perturbation procedures. Thus to place this theory in terms of a functional approach of the type developed here so as to give a self-consistent formalism, we need to develop a stationary action principle to enunciate the appropriate version of Theorem 2 given above. This has been achieved recently [19] using the Liouvillean quantum dynamics approach. In this theory, there is a natural doubling of the operators defined in Hilbert space, and correspondingly it leads to results in conformity with the nonequilibrium matrix Green-function theory of DuBois. Besides the advantage of the existence of the stationary action principle in this theory, the given initial condition that the system is in thermodynamic equilibrium, leading to the specification of the four-current and four-vector field averages at the initial time, are themselves derived in this theory from the equilibrium functional theory based on the free-energy minimum principle as in the earlier work of the author [4]. In this more general framework, the coupled matrix Green functions for both fields are obtained in terms of a modified functional $\tilde{\mathcal{B}}$ which is now constructed in terms of the density matrix in place of the state-vector average given above.

Kluger *et al.* [13] consider the problem of fermion pair production in a strong electric field. Here the quantum back action in spinor QED is set up and solved in semiclassical mean-field approximation for a homogeneous and time-dependent electric field. They apply the method of adiabatic regularization to the Dirac equation in order to renormalize the expectation value of the current operator and derive a finite coupled set of ordinary differential equations for the time evolution of the system. We could employ this technique to examine the solutions of Eqs. (19) and (20) with the appropriate redefinition of the current in Eq. (19a) to include the states both above and below the Fermi energy, so as to incorporate pair production processes. We would employ leading-order terms to evaluate the functional, Eq. (19c), so that the system of equations thus obtained is on par with those set up by Kluger *et al.* It seems to us that such a procedure may be a useful way to include aspects of self-consistency inherent in the functional scheme.

Another possible application of our theory is to develop the time-dependent optimized potential in a manner similar to that proposed by Ullrich and Gross [20]. This is for the purpose of analyzing the effects of ultrashort laser pulses of very high intensity on atoms placed in the focus of such a laser pulse. The new phenomena observed cannot be explained by means of perturbation theory and, in principle, a scheme such as ours should be of use. The work of Ulrich and Gross is designed to examine the nonrelativistic regime of the potential generated in this system, and does not examine the *back action* on the radiation field. Our formulation enables such an examination because the functional given by Eq. (19c) serves to generate the needed input for both the electron and electrodynamic equations.

V. FUTURE PLANS AND CONCLUDING REMARKS

In order to give a flavor of the Green-function formulation in the functional theory, which is useful in generating diagrammatic approximation schemes, it suffices to state here the relevant equations and relate them to those considered in Ref. [9]. The electron Green function associated with Eq. (19) is

$$G^{-1}(\vec{r}t;\vec{r}'t')=G_0^{-1}(\vec{r}t;\vec{r}'t')+V_{\text{eff}}[G,\mathcal{D}]\ , \tag{22}$$

$$V_{\text{eff}}[G,\mathcal{D}]=\gamma_\mu\left[A^\mu(\vec{r}t)+\frac{\delta\tilde{B}[J,A]}{\delta J_\mu(\vec{r}t)}\right]\delta(\vec{r}-\vec{r}')\delta(t-t')\ ,$$

and the dyadic Green function for the components of the em fields is

$$\mathcal{D}^{-1}=\mathcal{D}_0^{-1}+\Sigma_{\text{eff}}\ , \tag{23}$$

$$\Sigma_{\text{eff}_{\mu\nu}}=\Pi_{\mu\nu}+\frac{\delta^2\tilde{\mathcal{B}}}{\delta\mathcal{A}_\mu\delta\mathcal{A}_\nu}\ ,\quad \Pi_{\mu\nu}=\frac{\delta J_\mu}{\delta A_\nu}\ .$$

In Eq. (22), the first term corresponds to the usual noninteracting Green function, and the second term is the effective electron self-energy which is here local in space and time but in general a nonlinear functional of the currents and fields, containing contributions due to both the electron interactions and the electrodynamic coupling contributions, in contrast to the nonlocal self-energy in Ref. [9]. In Eq. (23), the first term is the noninteracting em Green function; the second term is the effective self-energy of the em fields consisting of two parts; Π, representing the polarization contributions, and a second piece containing further interaction-correlation contributions. As usual we have the definition $\mathcal{D}_{\mu\nu}=c\delta A_\mu/4\pi\delta j_\nu^{\text{ext}}$. It is clear that the central functional of importance is $\tilde{\mathcal{B}}$, which contains salient information con-

cerning the mutual correlations and interactions among the fields. From Eq. (19c), this functional needs further investigation in the future; it is sufficient here to note that by picking leading-order diagrams, one may set up some starting functionals, yielding a self-consistent scheme. It also should be remarked that in constructing this functional, all the field theory formalism has to be incorporated, so that the contributions of renormalizations, etc. are contained therein. (Recall that in the earlier Dirac electron theory of Refs. [4], [7], and [10], such constructions were given.)

In summary, here we have presented a time-dependent functional scheme for the coupled matter-electromagnetic field systems, where the two fields are treated on equal footing in a self-consistent manner. This theory is designed to deal with condensed-matter systems, but require modifications for applications in other situations as was outlined in Sec. IV. To our knowledge, such a theory has not been considered before in the literature and may be considered as the functional formulation of the usual interacting fields, such as those given in Refs. [8] and [9]. We have also indicated the generalization of our formalism to nonequilibrium situations.

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