Quantum electrodynamical time-dependent density-functional theory for many-electron systems on a lattice

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We present a rigorous formulation of the time-dependent density-functional theory for interacting lattice electrons strongly coupled to cavity photons. We start with an example of one particle on a Hubbard dimer coupled to a single photonic mode, which is equivalent to the single mode spin-boson model or the quantum Rabi model. For this system we prove that the electron-photon wave function is a unique functional of the electronic density and the expectation value of the photonic coordinate, provided the initial state and the density satisfy a set of well defined conditions. Then we generalize the formalism to many interacting electrons on a lattice coupled to multiple photonic modes and prove the general mapping theorem. We also show that for a system evolving from the ground state of a lattice Hamiltonian any density with a continuous second time derivative is locally v representable.

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I. INTRODUCTION

Time-dependent density-functional theory (TDDFT) is a formulation of the quantum many-body problem based on the one-to-one map from the time-dependent density to the driving external potential [1–3]. The main practical outcome of this map, which underlies the popularity of TDDFT, is a possibility to reproduce the dynamics of the exact density in the interacting many-body system by solving an auxiliary problem for a noninteracting Kohn-Sham (KS) system driven by a properly adjusted self-consistent potential. This dramatically reduces the complexity of the problem and necessary computational resource to study the dynamics of many-particle systems.

The standard TDDFT assumes that the system is driven by a classical time-dependent electromagnetic field [2,3]. This approach is indeed sufficient for most typical situations in quantum chemistry and condensed matter physics. However, in the recent years, with the impressive progress in the fields of cavity and circuit quantum electrodynamics (QED) it has been made possible to experimentally study systems interacting strongly with quantum light, like atoms in optical cavity [4–6], superconducting qubits and quantum dots [7–10], trapped ions [11], and molecules interacting with cavity photons [12–14].

Recently a generalization of TDDFT for quantum many-electron systems coupled to cavity photons has been proposed [15,16]. This theory, which can be named QED-TDDFT, relies on a generalized mapping theorem stating that there exists a unique map from the time-dependent electronic density and the expectation value of the photonic field to the total electron-photon wave function. In Ref. [15] the uniqueness of this generalized mapping has been demonstrated using the Taylor expansion technique under the standard in TDDFT assumption of analyticity in time [1,17]. The question of existence of the density-to-potential map, which is known in DFT as the v-representability problem, is much more difficult. In fact, in

the standard TDDFT for continuum systems this question is still not fully resolved, although a significant progress has been made recently [18].

Currently a complete and rigorous formulation of TDDFT, including the resolution of the v-representability problem, is available for lattice many-body systems [19,20]. The aim of the present paper is to extend the uniqueness and existence theorems of the lattice TDDFT to systems strongly interacting with a quantized electromagnetic field.

To make the idea of the proof more transparent we start with the simplest nontrivial system of one electron on a two-site lattice (a Hubbard dimer) coupled to a single photonic mode. It is worth noting that formulation of TDDFT for this system has its own value. Indeed, the dimer coupled to a quantum Bose field is (unitary) equivalent to such well known and popular models as the quantum Rabi model and the spin-boson model [21–23] which have a wide variety of applications ranging from quantum optics [24] and molecular physics [25] to the magnetic resonance in solid state physics [26]. There is also a natural connection to the Dicke model [27,28]. For this system we prove that, provided some well-defined conditions are fulfilled, there exists a unique mapping from the time-dependent on-site density and the expectation value of the bosonic coordinate to the wave function and the external deriving potentials. Afterwards we extend the QED-TDDFT mapping theorem to the general case of N interacting electrons on an M-site lattice coupled to multiple photonic modes. We also prove that, similar to the standard lattice TDDFT [20], the local existence/v representability is guaranteed if the dynamics starts from the ground state of a lattice Hamiltonian.

The structure of the paper is the following. In Sec. II we present a complete formulation of QED-TDDFT for the Hubbard dimer coupled to a single photonic mode. We derive the equation of motion for the expectation value of the field and the force balance equation and construct the corresponding universal nonlinear Schrödinger equation (NLSE). Then we prove the mapping theorem of QED-TDDFT for this model by applying the known results from the theory

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of semilinear partial differential equations (PDE) [29,30]. In Sec. III we generalize the formalism to the system of many particles on a many-site lattice which is coupled to multiple photonic modes. We derive the corresponding NLSE to the many-body system and then formulate and prove the general existence and uniqueness theorem for the lattice QED-TDDFT. Section IV presents a practically important case of a system evolving from its ground state. The main outcome of this section is the theorem of a local v representability for the initial ground state. In the Conclusion we summarize our results.

II. QED-TDDFT FOR A HUBBARD DIMER COUPLED TO A SINGLE PHOTONIC MODE

To make our approach more transparent and clear we consider first a simple system of one quantum particle on a two-site lattice, which is coupled to a single mode photonic field. The state of the system at time t is characterized by the electron-photon wave function $\psi_i(p;t) = \langle i, p | \Psi(t) \rangle$, where the index $i = \{1, 2\}$ corresponds to the particle coordinate and takes values on the lattice sites, and the real continuum variable p describes the photonic degree of freedom.

In this model the electronic density is coupled to the external on-site potential $v_i(t)$ which acts on the individual sites, while the photonic subsystem can be driven (excited) independently by an external time-dependent current $J_{ex}(t)$. Assuming that the wavelength of the photon field is much larger than the size of the system, we adopt the dipole approximation [31]. It is convenient to use the length gauge for the photon field. In this case the photon variable p is associated to the electric field which is coupled to the electron dipole moment [15,16]. Figure 1 shows a schematic view of a two-site lattice in a quantum cavity.
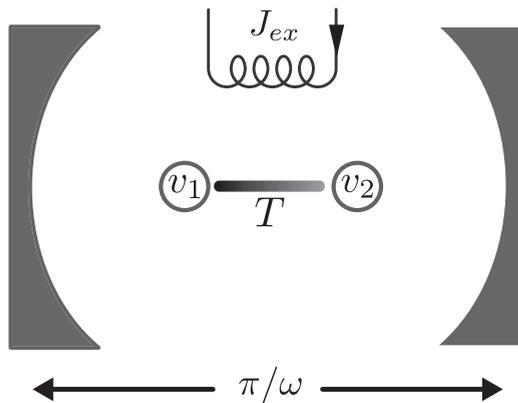

FIG. 1. Schematic view of a two-site lattice in a cavity. The electron, which can tunnel from one site to the other with the hopping rate T, experiences the on-site potential $v_i(t)$ specific to that site. The photonic field in the cavity is driven by a time-dependent external current $J_{ex}(t)$. The wavelength of the electromagnetic field $2\pi/\omega$ is proportional to the cavity size and assumed to be much larger than the lattice size, so that we can adopt the dipole approximation for the electron-photon interaction.

The following time-dependent Schrödinger equation governs the time evolution of the electron-photon wave function $\psi_i(p;t)$ from a given initial state $\psi_i(p,t_0)$

$$i\partial_t \psi_1(p;t) = -T\psi_2(p;t)$$
$$+ \left(\frac{-\partial_p^2}{2} + \frac{\omega^2 p^2}{2} + J_{ex}(t)p + \lambda p + v_1(t) \right)$$
$$\times \psi_1(p;t), \tag{1a}$$

$$i\partial_t \psi_2(p;t) = -T\psi_1(p;t)$$
$$+ \left(\frac{-\partial_p^2}{2} + \frac{\omega^2 p^2}{2} + J_{ex}(t)p - \lambda p + v_2(t) \right)$$
$$\times \psi_2(p;t), \tag{1b}$$

where the real coefficient T corresponds to the rate of hopping from one site to the other, ω is the frequency of the photon mode, and λ is the electron-photon coupling constant (see Fig. 1).

Formally Eqs. (1) describe a driven two-level system coupled to a quantum harmonic oscillator. Because of the gauge invariance the physics is not changed if we add to the potential a global time-dependent constant. Therefore without loss of generality we can adopt the gauge condition $v_1 + v_2 = 0$ and define the on-site potential as follows: $v(t) = v_1(t) = -v_2(t)$. With this definition the Hamiltonian in Eq. (1) takes to form

$$\hat{H}(t) = -T\hat{\sigma}_x + v(t)\hat{\sigma}_z + \lambda p\hat{\sigma}_z - \frac{\partial_p^2}{2} + \frac{\omega^2 p^2}{2} + J_{ex}(t)p. \tag{2}$$

$\hat{\sigma}_x$ and $\hat{\sigma}_z$ are the Pauli matrices, and a 2×2 unit matrix is assumed in the last three terms. The first two terms in Eq. (2) correspond to a two-level system (spin 1/2), while the last three terms describe a driven harmonic oscillator. Finally the third term in Eq. (2) is a linear coupling between the discrete and continuous variables. It is now clear the Eq. (1) is equivalent to the Schrödinger equation for the Rabi model or single mode spin-boson model [21–23]. Therefore, the subsequent discussion and all results of this section are directly applicable to these models. We also note that a detailed derivation of Hamiltonian Eq. (2) for a nonrelativistic system in a cavity can be found in Ref. [16] (see Appendix E).

Let us now turn to the formulation of QED-TDDFT. In general all DFT-like approaches assume that the state of the system is uniquely determined by a small set of basic observables, such as the density in TDDFT, the current in TDCDFT. Below we prove a theorem which generalizes the lattice TDDFT of Ref. [20] to the system coupled to a quantum oscillatoric degree of freedom as defined in Eq. (1). Namely, we will prove that, provided some well defined conditions are fulfilled, the electron-photon wave function $\Psi(t)$ is uniquely determined by the on-site density n_i and the expectation value of the photonic coordinate $P = \langle p \rangle$.

In our formulation we follow the NLSE approach to TDDFT [19,20,32–34] and adopt the same general logic as in Ref. [20]. We start with defining the basic observables for our two-site model. The first basic variable is the on-site density n_i—the

number of particles on the site i,

$$n_i(t) = \int dp |\psi_i(p;t)|^2. \tag{3}$$

For the electron-photon system the second, photon-related variable is required. The most natural choice [15,16] is the expectation value P of the photonic coordinate p

$$P = \int dp (|\psi_1(p;t)|^2 + |\psi_2(p;t)|^2) p. \tag{4}$$

The next step is to find the equations which relate the basic observables, the density n_i and the field average P, to the external potentials, the on-site potential v_i and the external current J_{ex}. Therefore we proceed to deriving the equations of motion for the two fundamental variables.

In order to derive the relevant equation of motion for n_i we calculate the time derivative of (3) and then substitute the derivatives of the wave function from the Schrödinger equation (1). The result takes the following form:

$$\dot{n}_1(t) = -2 \,\text{Im}[T \rho_{12}(t)], \tag{5}$$

where $\dot{n} = \partial_t n$, and $\rho_{12}(t)$ is the density matrix,

$$\rho_{12} = \int \rho_{12}(p;t) dp = \int \psi_1^*(p;t) \psi_2(p;t) dp. \tag{6}$$

The conservation of the particles dictates that the change in the density in one site is equal to minus the change in the other site $\dot{n}_2 = 2 \,\text{Im} T \rho_{12}$. Obviously, Eq. (5) is a lattice version of the continuity equation for site 1. Since in the left-hand side of Eq. (5) we have the time derivative of the on-site density, the right-hand side should be identified with a current flowing along the link connecting the two sites

$$J_{12}(t) = 2 \,\text{Im}[T \rho_{12}(t)]. \tag{7}$$

Differentiating the continuity equation (5) with respect to time and replacing the derivative of the wave function from the Schrödinger equation we get an equation which connects the on-site density n_i to the on-site potential v_i

$$\ddot{n}_1(t) = -2T \left(\text{Re}[\rho_{12}](v_1(t) - v_2(t)) \right.$$
$$\left. + T(n_1 - n_2) + 2\lambda \int \text{Re}[\rho_{12}(p)] p \, dp \right). \tag{8}$$

Physically this equation can be interpreted as the (discrete) divergence of the force balance equation for the two-site model [20].

A special role of Eq. (8) for TDDFT follows from the fact that it explicitly relates the potential disbalance $v_1(t) - v_2(t)$ to the density $n_i(t)$ and its derivatives. Like before, the conservation of the particle imposes $\ddot{n}_2 = -\ddot{n}_1$. Hence the force balance equation for $n_2(t)$ is obtained from Eq. (8) by changing the sign in the right hand side.

It is worth noting that the coefficient of the potential disbalance, $v_1(t) - v_2(t)$, in the force balance equation (8) is the kinetic energy $k_{12} = 2T \,\text{Re}[\rho_{12}]$; therefore for the current J_{12} and kinetic energy k_{12} we have

$$K_{12} + i J_{12} = 2T \rho_{12}. \tag{9}$$

Importantly, Eq. (8) contains only the potential disbalance $v_1 - v_2$ which reflects the well known gauge redundancy of TDDFT. For a given density the force balance equation fixes the on-site potential up to a constant. In order to resolve this issue we fix the gauge by considering on-site potentials which sum up to zero $v_1 = -v_2 = v$. This can be interpreted as a switching from the whole two-dimensional space of all allowed potentials to the one-dimensional space of equivalence classes for physically distinct potentials.

Next, we need to derive a similar equation for P. So we differentiate (4) with respect to t and simplify the right hand side using the Schrödinger equation (1) and the result is as follows:

$$\dot{P} = \text{Im} \left[\int (\psi_1^* \partial_p \psi_1 + \psi_2^* \partial_p \psi_2) dp \right]. \tag{10}$$

For brevity we suppressed the explicit p and t dependence of the wave function.

By differentiating Eq. (10) with respect to time and again substituting the time derivatives from the Schrödinger equation (1) we get an equation which relates J_{ex} to P, $\ddot{P}$, and n_i

$$\ddot{P} = -\omega^2 P - \lambda(n_1 - n_2) - J_{\text{ex}}(t). \tag{11}$$

This equation is, in fact, the inhomogeneous Maxwell equation projected on the single photon mode [16].

In the next subsection we will use the force balance equation (8) and equation of motion (11) to analyze the existence of a TDDFT-like theory for a two-site lattice coupled to a photonic field.

Statement of the mathematical problem and the basic existence theorem

The standard TDDFT is based on the existence a one-to-one map between the time-dependent density and the external potential. In the case of the electron-photon system the map is slightly different. Here the two basic observables, the on-site density n_i and the expectation value of the field P, are mapped to the two external fields, the on-site potential $v(t)$ and the external current $J_{\text{ex}}(t)$.

Equations (1), (3), and (4) uniquely determine the instantaneous wave function $\Psi(t)$, the on-site density n_i, and the field average P as functionals of the initial state Ψ_0, the on-site potential $v(t)$, and the external current $J_{\text{ex}}(t)$. This defines a unique "direct" map $\{\Psi_0, v, J_{\text{ext}}\} \rightarrow \{\Psi, n, P\}$ that is related to the standard direct quantum mechanical problem—reconstruction of the wave function $\Psi(t)$ from the initial data and the external potentials.

The TDDFT formalism for this problem relies on the existence of a unique map from the density n, the field average P and Ψ_0 to the potential v, the external current J_{ext}, and the wave function Ψ. In other words, TDDFT assumes the existence of a unique solution to the "inverse" problem of reconstructing the state $\Psi(t)$ and the potentials from the given observables and the initial data. In the following we will refer to the corresponding map $\{\Psi_0, n, P\} \rightarrow \{\Psi, v, J_{\text{ext}}\}$ as the "inverse map" to indicate that it is related to the above inverse problem. To prove the inverse map we follow the NLSE approach to TDDFT-type theories [19,20,32–34].

Assuming $n_i(t)$ and $P(t)$ are given functions of time, we express v and J_{ex} from the equations (8) and (11) as follows:

$$v = -\frac{\ddot{n}_1 + 2T^2(n_1 - n_2) + 4T\lambda \int \text{Re}[\rho_{12}(p)]p\, dp}{4T\,\text{Re}[\rho_{12}]}, \quad (12)$$

$$J_{ex} = -\ddot{P} - \omega^2 P - \lambda(n_1 - n_2), \quad (13)$$

where we assumed that $\text{Re}[\rho_{12}] \neq 0$.

We note that at any time, including the initial time $t = t_0$, the given density has to be consistent with the wave function. At $t = t_0$ this means that the right hand sides of Eq. (3) evaluated at the initial wave function Ψ_0 have to be equal to $n_i(t_0)$ in the left hand side. The same follows for the first derivative of the density $\dot{n}_i$ and the field average P and its first derivative $\dot{P}$. All of them should be consistent with the initial state Ψ_0 through Eqs. (5), (4), and (10), respectively. The consistency conditions which should be fulfilled are the following:

$$n_i(t_0) = \int dp\, |\psi_i(p; t_0)|^2, \quad (14a)$$

$$\dot{n}_1(t_0) = -2\,\text{Im}[T\rho_{12}(t_0)], \quad (14b)$$

$$P(t_0) = \int dp\, p(|\psi_1(p; t_0)|^2 + |\psi_2(p; t_0)|^2), \quad (14c)$$

$$\dot{P}(t_0) = \text{Im}\left[\int dp(\psi_1^*(p; t_0)\partial_p\psi_1(p; t_0) + \psi_2^*(p; t_0)\partial_p\psi_2(p; t_0)) \right]. \quad (14d)$$

The on-site potential v of Eq. (12) and the external current J_{ex} of Eq. (13) can be substituted as functionals of n, P, and Ψ into the Schrödinger equation (1). The result is a universal NLSE in which the Hamiltonian is a function of the instantaneous wave function and the (given) basic variables

$$i\partial_t \Psi(t) = H[n, P, \Psi]\Psi(t). \quad (15)$$

Now the question of existence of a unique QED-TDDFT map $\{\Psi_0, n_i, P\} \rightarrow \{\Psi, v, J_{ext}\}$ can be formulated mathematically as the problem of existence of a unique solution to NLSE (15) with given $n_i(t)$, $P(t)$, and Ψ_0.

Theorem 1. (Existence of QED-TDDFT for a Hubbard dimer coupled to a photonic mode.) Assume that the on-site density $n_i(t)$ is a positive, continuous function of time, which has a continuous second derivative and adds up to unity, $n_1(t) + n_2(t) = 1$. Consider $P(t)$ which is a continuous function of time with a continuous second derivative. Let Ω be a subset of the Hilbert space where $\text{Re}[\rho_{12}] \neq 0$. If the initial state $\Psi_0 \in \Omega$, and the consistency conditions of Eqs. (14) hold true, then:

(*i*) There is an interval around t_0 in which NLSE (15) has a unique solution and, therefore, there exists a unique map $\{\Psi_0, n_i, P\} \rightarrow \{\Psi, v, J_{ext}\}$.

(*ii*) The solutions (i.e., the QED-TDDFT map) are not global in time if at some $t^* > t_0$ the boundary of Ω is reached.

Proof. By the condition of the theorem $\Psi_0 \in \Omega$ where $\text{Re}[\rho] \neq 0$. Therefore, the on-site potential v can be expressed in terms of the density and the wave function as given by (12), and the Hamiltonian $\hat{H}[n, P, \Psi]$ in the universal NLSE is well defined.

Let us rewrite NLSE (15) in the following form:

$$i\partial_t \Psi = (\hat{H}_0 + \hat{H}_1[n, P, \Psi])\Psi, \quad (16)$$

where $\hat{H}_0$ is the time-independent (linear) part of the Hamiltonian,

$$\hat{H}_0 = -\tfrac{1}{2}\partial_p^2 + \tfrac{1}{2}\omega^2 p^2 + \lambda p\hat{\sigma}_z - T\hat{\sigma}_x, \quad (17)$$

and $\hat{H}_1$ contains all time-dependent, in particular non-linear, terms,

$$\hat{H}_1[n, P, \Psi] = J_{ex}[n, P]p + v[n, P, \Psi]\hat{\sigma}_z. \quad (18)$$

Here $J_{ex}[n, P]$ and $v[n, P, \Psi]$ are defined by Eqs. (13) and (12), respectively.

Since $\hat{H}_0$ is the Hamiltonian of the static shifted harmonic oscillator it defines a continuous propagator in the Hilbert space of square integrable functions. Therefore, Eq. (16) can be transformed to the following integral equation:

$$\Psi(t) = e^{-i\hat{H}_0(t-t_0)}\Psi_0$$
$$- i\int_{t_0}^t e^{-i\hat{H}_0(t-s)}\hat{H}_1[n(s), P(s), \Psi(s)]\Psi(s)ds. \quad (19)$$

To prove the existence of solutions to this equation we can use well established theorems from the theory of quasilinear PDE [29,30]. In particular, we apply the following result. Consider an integral equation of the form

$$u(t) = W(t, t_0)u_0 + \int_{t_0}^t W(t, s)K_s(u(s))ds, \quad (20)$$

where $W(t, s)$ is a continuous linear propagator on $T = [t_0, \infty)$ and the kernel $K_t(u)$ is a continuous function of time, which is locally Lipschitz in a Banach space $\mathcal{B}$. Then there is an interval $[t_0, t^*]$ where Eq. (20) has a unique continuous solution.

In our case we consider L^2 as the proper Banach space $\mathcal{B}$. The kernel $K_t(\Psi) = \hat{H}_1[n(t), P(t), \Psi]\Psi$ in Eq. (19) is continuous and Lipschitz in L^2 if $n(t)$, $\ddot{n}(t)$, $P(t)$, and $\dot{P}(t)$ are continuous functions of time, $\Psi \in \Omega$, $n_1, n_2 > 0$, $n_1 + n_2 = 1$ and the consistency conditions Eqs. (14) are fulfilled. Hence if all conditions of the theorem are satisfied Eq. (19) has a unique solution. Moreover, since in this case Ψ_0 is in the domain of H_0, $\Psi_0 \in D(H_0)$, there exists a unique differentiable (strong) solution of Eq. (19) which proves the statement (*i*) of the theorem.

The extension theorems for quasilinear PDE imply that the local solution cannot be extended beyond some maximal existence time $t^* > t_0$ only in two cases: first, at $t \rightarrow t^*$ the solution becomes unbounded or, second, at $t \rightarrow t^*$ it reaches the boundary of Ω. In our case the solution is guaranteed to be normalized and thus bounded. Therefore we are left only with the second possibility, which proves the statement (*ii*) and completes the proof of the theorem.

The above theorem generalizes the results of Ref. [16] where the uniqueness (but not the existence) of the map $\{\Psi_0, n_i, P\} \rightarrow \{\Psi, v, J_{ext}\}$ has been proven for analytic in time potentials using the standard Taylor expansion technique.

Theorem 1 can be straightforwardly generalized to the case of multiple photon modes. The only difference is that $\hat{H}_0$ in Eq. (17) becomes the Hamiltonian of a multidimensional shifted harmonic oscillator. The rest of the proof remains unchanged. This proves the existence of QED-TDDFT for

the spin-boson model in its standard form [22]. A less obvious generalization for the system of many interacting electrons on a many-site lattice is presented in the next section.

III. QED-TDDFT FOR MANY ELECTRONS ON MANY-SITE LATTICES INTERACTING WITH CAVITY PHOTONS

In the previous section we proved the QED-TDDFT existence theorem for a system of one electron on a two-site lattice coupled to a photonic mode. Below we generalize our results to the case of N interacting electrons on a M-site lattice coupled to L photonic modes. The state of the system is described by an electron-photon wave function $\psi(\mathbf{r}_1, \ldots, \mathbf{r}_N; \{p\})$ where coordinates $\mathbf{r}_i$ of the particles ($i = 1, 2, \ldots, N$) take values on the lattice sites and $\{p\}$ is the set of continuous coordinates describing the photonic (oscillatoric) degrees of freedom $\{p\} = \{p_1, p_2, \ldots, p_L\}$. Again we assume that the electronic subsystem is driven by classical on-site potentials $v(\mathbf{r}; t)$ and each photonic mode is coupled to corresponding external current $J_{\text{ex}}^\alpha(t)$. As usual, assuming that the size of the lattice is much smaller than the wavelength of the photon field, we describe the electron-photon coupling at the level of the dipole approximation with $\boldsymbol{\lambda}_\alpha$ being the coupling constant to the α photon.

The following time-dependent Schrödinger equation describes the time evolution of the system from the initial state $\psi_0(\mathbf{r}_1, \ldots, \mathbf{r}_N; \{p\})$

$$i\partial_t \psi(\mathbf{r}_1, \ldots, \mathbf{r}_N; \{p\})$$
$$= -\sum_{i=1}^{N} \sum_{\mathbf{x}_i} T_{\mathbf{r}_i, \mathbf{x}_i} \psi(\ldots, \mathbf{x}_i, \ldots; \{p\})$$
$$+ \sum_{i=1}^{N} v(\mathbf{r}_j; t) \psi(\mathbf{r}_1, \ldots, \mathbf{r}_N; \{p\})$$
$$+ \sum_{j>i} w_{\mathbf{r}_i, \mathbf{r}_j} \psi(\mathbf{r}_1, \ldots, \mathbf{r}_N; \{p\})$$
$$+ \sum_{\alpha=1}^{K} \left[-\frac{1}{2}\partial_p^2 + \frac{1}{2}\omega_\alpha^2 p_\alpha^2 + J_{\text{ex}}^\alpha(t) p_\alpha \right]$$
$$\times \psi(\mathbf{r}_1, \ldots, \mathbf{r}_N; \{p\})$$
$$+ \sum_{i=1}^{N} \sum_{\alpha=1}^{K} \boldsymbol{\lambda}_\alpha \cdot \mathbf{r}_i \, p_\alpha \psi(\mathbf{r}_1, \ldots, \mathbf{r}_N; \{p\}), \quad (21)$$

where the real coefficients $T_{\mathbf{r}, \mathbf{r}'} = T_{\mathbf{r}', \mathbf{r}}$ correspond to the rate of hopping from site $\mathbf{r}$ to site $\mathbf{r}'$ (for definiteness we set $T_{\mathbf{r}, \mathbf{r}} = 0$), and $w_{\mathbf{r}, \mathbf{r}'}$ is the potential of a pairwise electron-electron interaction.

Following the logic of Sec. II we define the on-site density $n(\mathbf{r})$ and the expectation value of the field P_α for a mode α, which are the basic variables for the QED-TDDFT

$$n(\mathbf{r}) = N \sum_{\mathbf{r}_2, \ldots, \mathbf{r}_N} \int |\psi(\mathbf{r}, \mathbf{r}_2, \ldots, \mathbf{r}_N; \{p\})|^2 d\mathbf{p}, \quad (22)$$

$$P_\alpha = \sum_{\mathbf{r}_1, \ldots, \mathbf{r}_N} \int p_\alpha |\psi(\mathbf{r}, \ldots, \mathbf{r}_N; \{p\})|^2 d\mathbf{p}, \quad (23)$$

where $d\mathbf{p} = dp_1 \cdots dp_L$.

Similar to the two-site case we derive the force balance equation by calculating the second derivative of the density (22) and using the Schrödinger equation (21) to simplify the terms with the time derivative of the wave function

$$\ddot{n}(\mathbf{r}) = 2\,\text{Re} \sum_{\mathbf{r}'} T_{\mathbf{r}, \mathbf{r}'} \rho(\mathbf{r}, \mathbf{r}')(v(\mathbf{r}'; t) - v(\mathbf{r}; t))$$
$$+ q(\mathbf{r}; t) + f(\mathbf{r}; t), \quad (24)$$

where $q(\mathbf{r}; t)$ is the lattice divergence of the internal forces

$$q(\mathbf{r}; t) = -2\,\text{Re} \sum_{\mathbf{r}', \mathbf{r}''} T_{\mathbf{r}, \mathbf{r}'} [T_{\mathbf{r}', \mathbf{r}''} \rho(\mathbf{r}, \mathbf{r}'') - T_{\mathbf{r}, \mathbf{r}''} \rho(\mathbf{r}', \mathbf{r}'')$$
$$+ \rho_2(\mathbf{r}, \mathbf{r}'', \mathbf{r}')(w_{\mathbf{r}, \mathbf{r}''} - w_{\mathbf{r}', \mathbf{r}''})], \quad (25)$$

and $f(\mathbf{r}; t)$ is the force exerted on electrons from the photonic subsystem

$$f(\mathbf{r}; t) = 2\,\text{Re} \sum_{\alpha} \sum_{\mathbf{r}'} T_{\mathbf{r}, \mathbf{r}'} \boldsymbol{\lambda}_\alpha \cdot (\mathbf{r}' - \mathbf{r}) \int p_\alpha \rho(\mathbf{r}, \mathbf{r}'; p_\alpha) dp_\alpha. \quad (26)$$

Here $\rho(\mathbf{r}, \mathbf{r}')$ is the one-particle density matrix

$$\rho(\mathbf{r}, \mathbf{r}') = \int \rho(\mathbf{r}, \mathbf{r}'; p_\alpha) dp_\alpha$$
$$= N \sum_{\mathbf{r}_2, \ldots, \mathbf{r}_N} \int \psi^*(\mathbf{r}, \mathbf{r}_2, \ldots, \mathbf{r}_N; \{p\})$$
$$\times \psi(\mathbf{r}', \mathbf{r}_2, \ldots, \mathbf{r}_N; \{p\}) d\mathbf{p} \quad (27)$$

and $\rho_2(\mathbf{r}, \mathbf{r}'', \mathbf{r}')$ is the two-particle density matrix

$$\rho_2(\mathbf{r}, \mathbf{r}'', \mathbf{r}') = N(N-1) \sum_{\mathbf{r}_3, \ldots, \mathbf{r}_N} \int [\psi^*(\mathbf{r}, \mathbf{r}'', \ldots, \mathbf{r}_N; \{p\})$$
$$\times \psi(\mathbf{r}', \mathbf{r}'', \ldots, \mathbf{r}_N; \{p\})] d\mathbf{p}. \quad (28)$$

The equation of motion for the field average P_α (23) is derived in the same manner as in Sec. II by calculating the second time derivative of P_α and using the Schrödinger equation (21),

$$\ddot{P}_\alpha = -\omega_\alpha^2 P_\alpha - J_{\text{ex}}^\alpha - \boldsymbol{\lambda}_\alpha \cdot \mathbf{d}, \quad (29)$$

where $\mathbf{d}$ is the total dipole moment of the N-electron system

$$\mathbf{d} = \sum_{\mathbf{r}} \mathbf{r} n(\mathbf{r}). \quad (30)$$

The existence of QED-TDDFT is equivalent to the existence of the inverse map $\{\Psi_0, n(\mathbf{r}), P_\alpha\} \to \{\Psi, v, J_{\text{ext}}^\alpha\}$. To study this map we compile the universal NLSE by expressing the on-site potential $v(\mathbf{r})$ and the external current J_{ext}^α in terms of the fundamental observables $n(\mathbf{r})$ and P_α, and the wave function Ψ.

To find the current J_{ext}^α as a functional of the field average P_α and the density $n(\mathbf{r})$ we only need to rearrange Eq. (29)

$$J_{\text{ex}}^\alpha = -(\ddot{P}_\alpha + \omega_\alpha^2 P_\alpha + \boldsymbol{\lambda}_\alpha \cdot \mathbf{d}). \quad (31)$$

The problem of finding the potential $v(\mathbf{r})$ as a functional of $n(\mathbf{r})$ and Ψ is more involved [20] as we need to solve the system of

M linear equations, Eq. (24), for $v(\mathbf{r})$. Let us first rewrite (24) in a matrix form as follows:

$$\hat{K}[\Psi]V = S[\ddot{n}, \Psi], \qquad (32)$$

where $\hat{K}$ is a real symmetric $M \times M$ matrix with elements

$$k_{\mathbf{r},\mathbf{r}'}[\Psi] = 2\,\mathrm{Re}\left[T_{\mathbf{r},\mathbf{r}'}\rho(\mathbf{r},\mathbf{r}') - \delta_{\mathbf{r},\mathbf{r}'}\sum_{\mathbf{r}''}T_{\mathbf{r},\mathbf{r}''}\rho(\mathbf{r},\mathbf{r}'')\right] \qquad (33)$$

and V and S are M-dimensional vectors with components

$$v_{\mathbf{r}} = v(\mathbf{r}), \qquad (34a)$$

$$s_{\mathbf{r}}[\ddot{n}, \Psi] = -\ddot{n}(\mathbf{r}) - q[\Psi](\mathbf{r}) - f[\Psi](\mathbf{r}). \qquad (34b)$$

The problem of inverting (solving for $v(\mathbf{r})$) the force balance equation (32) for a general lattice has been analyzed in Ref. [20] in the context of the standard electronic TDDFT. The same argumentation regarding the properties of the matrix $\hat{K}$ is applicable in the present case. Solving Eq. (24) for the on-site potential $v(\mathbf{r})$ is equivalent to multiplying both sides of Eq. (32) by inverse of the $\hat{K}$ matrix. Therefore, the matrix $\hat{K}$ must be nondegenerate. At this point it is worth noting that because of the gauge invariance $\hat{K}$ matrix (33) always has at least one zero eigenvalue that corresponds to a space-constant eigenvector. Therefore, if $\mathcal{V}$ is the M-dimensional space of lattice potentials $v(\mathbf{r})$, then the invertibility/nondegeneracy of $\hat{K}$ should always refer to the invertibility in an $(M-1)$-dimensional subspace of $\mathcal{V}$, which is orthogonal to a constant vector $v_C(\mathbf{r}) = C$. In more physical terms this means that the force balance equation (33) determines the self-consistent potential $v[n, \Psi](\mathbf{r})$ only up to an arbitrary constant, like Eq. (8) in Sec. II. Therefore, in the orthogonal subspace of $\mathcal{V}$ we have

$$V = \hat{K}^{-1}S, \qquad (35)$$

where by $\hat{K}^{-1}$ we mean inversion in the subspace of $\mathcal{V}$. Equation (35) is the required functional $v[n, \Psi](\mathbf{r})$, which can be used to construct the universal NLSE.

Finally, like in the two-site case (see Sec. II) the initial sate Ψ_0, the density $n(\mathbf{r})$, and the field average P_α should satisfy the consistency conditions at $t = t_0$

$$n(\mathbf{r}; t_0) = N\sum_{\mathbf{r}_2,\ldots,\mathbf{r}_N}\int |\psi_0(\mathbf{r},\ldots,\mathbf{r}_N;\{p\})|^2 d\mathbf{p}, \qquad (36a)$$

$$\dot{n}(\mathbf{r}; t_0) = -2\,\mathrm{Im}\left[\sum_{\mathbf{r}'}T_{\mathbf{r},\mathbf{r}'}\rho_0(\mathbf{r},\mathbf{r}')\right], \qquad (36b)$$

$$P_\alpha(t_0) = \sum_{\mathbf{r}_1,\ldots,\mathbf{r}_N}\int p_\alpha|\psi_0(\mathbf{r}_1,\ldots,\mathbf{r}_N;\{p\})|^2 d\mathbf{p}, \qquad (36c)$$

$$\dot{P}_\alpha(t_0) = \mathrm{Im}\sum_{\mathbf{r}_1,\ldots,\mathbf{r}_N}\int [\psi_0^*(\mathbf{r}_1,\ldots,\mathbf{r}_N;\{p\})$$
$$\times \partial_{p_\alpha}\psi_0(\mathbf{r},\ldots,\mathbf{r}_N;\{p\})]d\mathbf{p}. \qquad (36d)$$

By substituting the on-site potential $v(\mathbf{r})$ from Eq. (35), and the field average P_α from Eq. (31) into the Schrödinger equation (21) we find the proper NLSE

$$i\partial_t\Psi(t) = H[n, P, \Psi]\Psi(t), \qquad (37)$$

which we use to prove the existence of the unique inverse map $\{\Psi_0, n(\mathbf{r}), P_\alpha\} \to \{\Psi, v(\mathbf{r}), J_{\mathrm{ext}}^\alpha\}$ and thus the existence of the QED-TDDFT in a close analogy with Theorem 1.

Theorem 2. (Existence of the QED-TDDFT for lattice systems coupled to cavity photons.) Assume that a given time-dependent density $n(\mathbf{r}; t)$ is non-negative on each lattice site, sums up to the number of particles N, and has a continuous second time derivative $\ddot{n}(\mathbf{r}; t)$. Also assume that $P_\alpha(t)$ is a continuous function of t and has a continuous second time derivative $\ddot{P}_\alpha(t)$. Let Ω be a subset of the N-particle Hilbert space $\mathcal{H}$ where the matrix $\hat{K}[\Psi]$ (33) has only one zero eigenvalue corresponding to the space-constant vector. If the initial state $\Psi_0 \in \Omega$, and at time t_0 the consistency conditions of Eq. (36) are fulfilled, then:

(i) There is a time interval around t_0 where the many-body NLSE (37) has a unique solution that defines the wave function $\Psi(t)$, the external potentials $v(t)$ and $J_{\mathrm{ext}}^\alpha(t)$ as unique functionals of the density $n(\mathbf{r}; t)$, field average P_α, and the initial state Ψ_0.

(ii) The solution of item (i) is not global in time if and only if at some maximal existence time $t^* > t_0$ the boundary of Ω is reached.

The proof of this theorem goes along the same lines as the proof of Theorem 1 in Sec. II. We transform NLSE (37) to a multidimensional integral equation similar to (19) and then apply the general existence results [29,30] for equations of the type of Eq. (20) to show that the statements (i) and (ii) are in fact true. We skip the details as the procedure is mostly a straightforward repetition of the proof presented in Sec. II.

IV. TIME-DEPENDENT v REPRESENTABILITY FOR A SYSTEM EVOLVING FROM THE GROUND STATE

In this section we will show that the ground state of a quite general lattice Hamiltonian belongs to the v-representability subset Ω. This implies the map $\{\Psi_0, n, P_\alpha\} \to \{\Psi, v, J_{\mathrm{ext}}^\alpha\}$ is guaranteed to exist if the dynamics starts from the ground state. The main theorem of this section is a generalization of Theorem 2 in Ref. [20].

Consider the following lattice Hamiltonian of many mutually interacting electrons coupled to photonic modes:

$$\hat{H}_{\alpha,\beta,\gamma} = (\hat{T} + \hat{V} + \alpha\hat{W}_{e\text{-}e}) \otimes \hat{\mathbb{I}}_{\mathrm{ph}} + \hat{\mathbb{I}}_e \otimes \hat{H}_{\mathrm{ph}} + \beta H_{e\text{-}\mathrm{ph}}, \qquad (38)$$

where $\hat{T}$ is the usual lattice operator of the kinetic energy, $\hat{V}$ corresponds to the interaction with a local external potential, $\hat{W}$ describes the electron-electron interaction, $\hat{H}_{\mathrm{ph}}$ is the photonic Hamiltonian, and $H_{e\text{-}\mathrm{ph}}$ is the Hamiltonian for the interaction between electrons and the photon modes, $\hat{\mathbb{I}}_{\mathrm{ph}}$ and $\hat{\mathbb{I}}_e$ are, respectively, the unit matrices in the photonic and the electronic sectors of the Hilbert space, and α and β are real coefficients.

Here we demonstrate that the ground state of the Hamiltonian (38), for any $\alpha, \beta \in \mathbb{R}$ and any on-site potential, belongs to the v-representability subset Ω if all terms in Eq. (38) except $\hat{T}$ commute with the density operator $\hat{n}_{\mathbf{r}}$. The proof of this quite general statement closely follows the proof of the Theorem 2 in Ref. [20]. Therefore, below we only briefly go through the main line of arguments.

Assume that $\Psi_k = |k\rangle$ form a complete set of eigenstates for the Hamiltonian (38) and let $\Psi_0 = |0\rangle$ be the ground state. We will show that the matrix $\hat{K}[\Psi_0]$ evaluated at the ground state is strictly negative definite in the subspace of potentials that are orthogonal to a space-constant vector V_C. That is,

$$V^T \hat{K}[\Psi_0] V \equiv \sum_{\mathbf{r},\mathbf{r}'} v(\mathbf{r}) k_{\mathbf{r},\mathbf{r}'} v(\mathbf{r}) < 0, \qquad (39)$$

for all M-dimensional vectors $V = \{v(\mathbf{r})\}$ which are orthogonal to the spatially constant potential

$$V^T V_C = C \sum_{\mathbf{r}} v(\mathbf{r}) = 0, \qquad (40)$$

where V^T stands for a transposed vector. Therefore, $\hat{K}[\Psi_0]$ is nondegenerate in the subspace orthogonal the to constant potentials.

Using the f-sum rule and the spectral representation of the density-density response function (see, for example, Ref. [35]) one can represent the elements of $\hat{K}$-matrix Eq. (33) as follows (see Ref. [20] for details):

$$k_{\mathbf{r},\mathbf{r}'}[\Psi_0] = -4 \operatorname{Re} \sum_k \omega_{k0} \langle 0|\hat{n}_{\mathbf{r}}|k\rangle \langle k|\hat{n}_{\mathbf{r}'}|0\rangle, \qquad (41)$$

where $\omega_{k0} = E_k - E_0$ is the excitation energy of the system from the ground state to the state k.

Substituting $k_{\mathbf{r},\mathbf{r}'}$ of Eq. (41) into the left hand side of Eq. (39) we find the following result:

$$V^T \hat{K}[\Psi_0] V = -4 \sum_k \omega_{k0} \left| \sum_{\mathbf{r}} v(\mathbf{r}) \langle 0|\hat{n}_{\mathbf{r}}|k\rangle \right|^2$$
$$= -4 \sum_k \omega_{k0} |\langle 0|\hat{v}|k\rangle|^2 \leqslant 0, \qquad (42)$$

where $\hat{v}$ is an operator corresponding to the potential $v(\mathbf{r})$,

$$\hat{v} = \sum_{\mathbf{r}} v(\mathbf{r}) \hat{n}_{\mathbf{r}}. \qquad (43)$$

The equality in Eq. (42) holds only for a space-constant potential $v_C(\mathbf{r}) = C$. Indeed, since each term in the sum in Eq. (42) is non-negative, the result of summation is zero if and only if

$$\langle 0|\hat{v}|k\rangle = 0, \quad \text{for all } k \neq 0. \qquad (44)$$

Assuming that Eq. (44) is fulfilled and expanding the vector $\hat{v}|0\rangle$ in the complete set of states $\{|k\rangle\}$ we get

$$\hat{v}|0\rangle = \sum_k |k\rangle \langle k|\hat{v}|0\rangle = |0\rangle \langle 0|\hat{v}|0\rangle \equiv \lambda |0\rangle. \qquad (45)$$

Therefore, the condition of Eq. (44) implies that the ground state $|0\rangle$ is an eigenfunction of the operator $\hat{v}$. Since $\hat{v}$ corresponds to a local multiplicative one-particle potential this can happen only if the potential is spatially constant. Hence for all potentials which are orthogonal to a constant in a sense of Eq. (40) the strict inequality in Eq. (42) takes place. This means that matrix $\hat{K}[\Psi_0]$ is negative definite and thus invertible in the $(M-1)$-dimensional subspace of $\mathcal{V}$ orthogonal to a constant vector V_C. In other words, the ground state of N-particle system on a connected lattice does belong to the v-representability subset Ω. This result combined with the

general existence theorem of Sec. III proves the following particular version of the time-dependent v-representability theorem.

Theorem 3. Let the initial state Ψ_0 for a time-dependent many-body problem on a connected lattice corresponds to a ground state of a Hamiltonian of the form (38). Consider continuous positive density $n(\mathbf{r};t)$ and field average $P(t)$ which satisfy the consistency conditions of Eqs. (36) and have a continuous second time derivative. Then there is a finite interval around t_0 in which $n(\mathbf{r};t)$ and $P(t)$ can be reproduced uniquely by a time evolution of Schrödinger equation (21) with some time-dependent on-site potential $v_i(t)$ and external current $J_{\text{ex}}(t)$.

Note that Theorem 3 is valid for any Hamiltonian of the form of Eq. (38) as long as all the terms in the Hamiltonian, except the kinetic part, commute with the density operator $\hat{n}_{\mathbf{r}}$, and, therefore, do not contribute to the $\hat{K}$ matrix. An important special case is when the initial state is the interacting many-electron ground state which is decoupled from the photonic field, $\beta = 0$. In this case the ground state is a direct product of the electronic ground state and photonic ground state. Another practically relevant case of $\alpha = \beta = 0$ corresponds to the initial state in a form of the direct product of the noninteracting many-electron wave function (the Slater determinant) and the photonic vacuum. For all those cases the local v representability is guaranteed by the above Theorem 3.

V. CONCLUSION

In this work we extended the formalism of the lattice TDDFT [20] and presented a rigorous proof of the mapping theorem of QED-TDDFT for many-electron lattice systems coupled to quantized photonic modes. First we considered the simplest nontrivial model of a one-electron Hubbard dimer coupled to a single photonic mode, which is identical to the Rabi and spin-boson models. We identified a pair of basic variables describing the electronic and photonic degrees of freedom, and showed that the existence of the QED-TDDFT map is equivalent to the existence of a unique solution to a certain system of nonlinear partial differential equations (the universal NLSE). We proved that the Cauchy problem for this NLSE indeed has a unique solution and, therefore, the unique QED-TDDFT map exists, provided the basic variables have a continuous second time derivative and the initial state belongs to some well defined subset of the Hilbert space (the v-representability subset). Further we generalized the theory to many electrons and multiple photonic modes. We proved that the same QED-TDDFT mapping can be constructed for this generic interacting electron-photon system. Finally, we showed that the ground state of a quite general electron-photon lattice Hamiltonian belongs to the v-representability subset Ω of the Hilbert space. Therefore, if the system evolves from such a ground state the local v representability is always guaranteed.

The main difference and, in fact, the main mathematical difficulty of the present theory, as compared to the purely electronic lattice TDDFT [19,20], is the existence continuum variables describing photonic modes. As a result the Hilbert space becomes an infinite dimensional functional space, and the universal NLSE turns into a system of PDE. In a

certain sense the lattice QED-TDDFT is on halfway between the electronic lattice TDDFT and the usual TDDFT in the continuum space. Hopefully the present rigorous results will shed new light on remaining unresolved issues of TDDFT and thus deepen our understanding of this popular and practically important theory.

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