Implications of gauge-freedom for non-relativistic quantum electrodynamics

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We review gauge-freedom in quantum electrodynamics (QED) outside of textbook regimes. We emphasise that QED subsystems are defined relative to a choice of gauge. Each definition uses different gauge-invariant observables. We show that this relativity is only eliminated if a sufficient number of Markovian and weak-coupling approximations are employed. All physical predictions are gauge-invariant, including subsystem properties such as photon number and entanglement. However, subsystem properties naturally differ for different physical subsystems. Gauge-ambiguities arise not because it is unclear how to obtain gauge-invariant predictions, but because it is not always clear which physical observables are the most operationally relevant. The gauge-invariance of a prediction is necessary but not sufficient to ensure its operational relevance. We show that in controlling which gauge-invariant observables are used to define a material system, the choice of gauge affects the balance between the material system’s localisation and its electromagnetic dressing. We review various implications of subsystem gauge-relativity for deriving effective models, for describing time-dependent interactions, for photodetection theory, and for describing matter within a cavity.

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I. INTRODUCTION

Extreme light-matter interaction regimes have become an important topic in both applied and fundamental physics. Recent reviews [1–3] have focussed on effective models and new theoretical methods, which are required because standard weak-coupling quantum optics cannot be applied. Despite new methods, our understanding continues to be based on processes involving real and virtual bare quanta, which can vary significantly with the form of the model considered. Non-standard regimes are precisely where effective models that are only superficially motivated are liable to fall short. This necessitates an appraisal of the fundamental physics within such regimes via first principles, as will be the focus of the current article. We focus specifically on the implications of QED’s gauge-theoretic aspects.

Gauge-freedom in ultrastrong and deep-strong coupling QED has recently been investigated in a number of contexts [4–13]. Its importance lies in the fact that the fundamental gauge-relativity of QED subsystems can only be ignored in traditional regimes. This linear-space relativity is akin to that encountered in theories of space and time. For example, the time interval \( \Delta t_A \) between two events \( x \) and \( y \), as measured by a clock at rest in frame A does not predict the outcome \( \Delta t_B \) of measuring the time between \( x \) and \( y \) in a co-moving frame B. This is only so if the relativistic mixing incurred by the Lorentz transformation from A to B can be ignored so that \( \Delta t_A \approx \Delta t_B \). Otherwise, we have two different predictions, \( \Delta t_A \) and \( \Delta t_B \), for two different experiments; one in frame A and one in frame B. We do know however, which prediction corresponds to which experiment, that is, we always know which prediction is relevant. This is determined by the rest frame of the clock, i.e., it is determined by the apparatus. Suppose however, that we did not know which prediction matched which experiment. We would then have encountered an ambiguity.

In the same way that intervals in space and time can only be defined relative to an inertial frame in Minkowski spacetime, light and matter quantum subsystems can only be defined relative to a gauge-frame in Hilbert space. Traditional weak-coupling regimes are gauge-nonrelativistic, such that the gauge-relativity of quantum subsystems can be eliminated completely therein, using standard approximations. We demonstrate this directly in Sec. IV. Outside of these regimes there are many implications of QED’s subsystem gauge-relativity, not only the breakdown of gauge-invariance due to truncating the material subsystem to a finite number of energy levels [4–13]. Gauge-ambiguities have also been discussed in the context of time-dependent interactions [5, 7, 10], Dicke-model superradiance [6, 11], and photodetection theory [10].

Unlike in special relativity, where it is straightforward to identify which predictions of space and time intervals are relevant in which situations, in QED there are a number of conceptual subtleties regarding the identification of the most relevant theoretical subsystems. The problem is closely related to the interpretation of virtual processes and particles, an aspect of light-matter physics that already possesses a long history of theoretical studies predominantly confined so far to the weak-coupling regime. Such studies possess significant overlap with the quantum theory of measurement [14–22] as well as with the identification of local fields and causal signal propagation [23–32].

The primary purpose of the present article is to identify what gauge-ambiguities occur beyond the regimes traditionally considered in quantum optics and to clarify how they arise. In Sec. II we provide a rigorous derivation of arbitrary gauge non-relativistic QED using the principles of modern gauge-field theory, showing that the implications of gauge-freedom discussed in Secs. III onward are a fundamental feature. They are not in any way an artefact of approximations or simplifications. In particular, gauge-ambiguities arise not because it is unclear how to obtain gauge-invariant predictions, but because it is not always clear which gauge-invariant subsystems are operationally relevant.

In Sec. III we briefly review theoretical background for the implementation of material level truncations [4–9, 12, 13], noting that the resulting gauge non-invariance is prosaic, because it can always be avoided by avoiding the truncation. We emphasise the important difference between gauge non-invariance and gauge-ambiguities. We review various proposals for obtaining two-level models, along with their varying degree of accuracy in different regimes, as well as their significance for understanding gauge-ambiguities.

In Sec. IV we discuss time-dependent interactions. We first review the QED S-matrix formalism, noting that subsystem gauge-relativity can be completely ignored therein due to the adiabatic interaction-switching condition within its definition. This condition implies the strict conservation of the bare-energy \( h \) where \( H = h + V \)
is the full Hamiltonian and where the interaction $V$ is defined as the component that vanishes for vanishing coupling-strength. We show directly that conventional weak-coupling and Markovian approximations mimic the $S$-matrix by enforcing the conservation of $\hbar$. They thereby eliminate subsystem gauge-relativity. In contrast, it is shown that when describing non-Markovian and strong-coupling effects subsystem gauge-relativity cannot be ignored. The remainder of the article focusses on the important implications of this fact.

In Sec. V we consider photodetection theory. We emphasise that gauge-ambiguities arise because it is not always clear that any one definition of “photon” is always the most operationally relevant. For example, the Coulomb-gauge definition, which uses the transverse electric field $E_T$, has recently been adopted in ultrastrong-coupling light-matter physics literature [7, 10]. However, as has been known for some time, the natural lineshape prediction has been found to be closer to experiment if photons are defined relative to the multipolar-gauge [33–36]. This definition uses the gauge-invariant transverse displacement field $D_T$, which equals the total electric field $E$ away from the source and is therefore local, unlike $E_T$ [24–32].

We identify how the definitions of the subsystems, as controlled by the choice of gauge, are related to photodetection divergences [14, 15]. We calculate various local energy-densities, including virtual contributions, in the vicinity of a dipole, and determine the relation between subsystem gauge-relativity and electromagnetic dressing. We extend these considerations to cavity QED beyond standard regimes, and discuss how subsystem gauge-relativity relates to weak-measurements of intra-cavity subsystems and to ground state superradiance. We briefly mention outlook for predictions regarding extra-cavity fields. Finally, we summarise in Sec. VI.

II. SUBSYSTEM GAUGE-RELATIVITY

We begin with a pedagogical derivation of non-relativistic Hamiltonian QED in an arbitrary gauge. We then provide a rigorous derivation according to the principles of modern gauge-field theory. We define the gauge-principle, gauge-freedom, gauge-symmetry transformations, and gauge-fixing transformations. We show that all physical predictions are gauge-invariant. We introduce the notion of subsystem gauge-relativity and remark on its implications. These implications are discussed in detail in the remainder of the article.

A. Single-particle description in standard gauges

Consider a single charge $q$ with position $r$ bound to a fixed charge $-q$ at the origin 0 of our chosen inertial frame. The charge and current densities are

$$\rho(x) = -q\delta(x) + q\delta(x - r),$$

$$J(x) = q\hat{r}\delta(x - r),$$

such that $\dot{\rho} = -\nabla \cdot J$. These fields together with electric and magnetic fields $E$ and $B$, exhaustively assign material and electromagnetic properties to each event $x = (t, \mathbf{x})$ in spacetime. Scalar and vector potentials $A_0$ and $\mathbf{A}$ are defined by

$$E = -\nabla A_0 - \mathbf{A},$$

$$B = \nabla \times \mathbf{A},$$

which imply that the inhomogeneous Maxwell equations are automatically satisfied. The electric and magnetic fields are invariant under the gauge transformation

$$\mathbf{A}' = \mathbf{A} + \nabla \chi,$$

$$A_0' = A_0 - \partial_0 \chi$$

where $\chi$ is arbitrary.

Recall that the Helmholtz decomposition of a vector-field $\mathbf{V}$ into transverse and longitudinal fields, $\mathbf{V} = \mathbf{V}_T + \mathbf{V}_L$, is unique. The transverse and longitudinal components satisfy $\nabla \cdot \mathbf{V}_T = 0$ and $\nabla \times \mathbf{V}_L = 0$. Transverse and longitudinal delta-functions (dyadics) are defined by the non-local conditions

$$\mathbf{V}_{L,T}(x) = \int d^3x' \delta^{L,T}(x - x') \cdot \mathbf{V}(x').$$

Since the curl of the gradient is identically zero, the transverse vector potential $\mathbf{A}_T$ is gauge-invariant; $\mathbf{A}'_T = \mathbf{A}_T$. Thus, gauge-freedom is the freedom to choose the longitudinal vector potential $\mathbf{A}_L = \nabla \chi$ where $\mathbf{A} = \mathbf{A}_T + \nabla \chi$. The Coulomb-gauge is defined by the choice $\mathbf{A}_L = 0$, such that $\mathbf{A} = \mathbf{A}_T$. From Gauss’ law $\nabla \cdot \mathbf{E} = \rho$ and Eq. (3) it follows that in the Coulomb-gauge the scalar potential $A_0$ is the Coulomb potential, which is defined by

$$\phi(x) = \int d^3x' \frac{\rho(x')}{4\pi|x - x'|}.$$
where
\[
\chi_\alpha(x) = \int d^3x' \mathbf{g}_{T\alpha}(x', x) \cdot \mathbf{A}_T(x')
\]
(11)  \\
\[
\mathbf{g}_{T\alpha}(x', x) = -\alpha \int_0^1 d\lambda \mathbf{x} \cdot \delta^T(x' - \lambda \mathbf{x}).
\]
(12)

It is useful to define the polarisation field \( \mathbf{P} \) by the equation \(-\nabla \cdot \mathbf{P} = \rho \), which specifies \( \mathbf{P}_L \) uniquely, but leaves \( \mathbf{P}_T \) an essentially arbitrary transverse field. We are free to define the field \( \mathbf{P}_\alpha := \mathbf{P}_L + \mathbf{P}_{T\alpha} \) where \( \mathbf{P}_{T\alpha} \) is called the \( \alpha \)-gauge transverse polarisation defined by the condition
\[
\int d^3x \rho(x) \chi_\alpha(x) = -\int d^3x \mathbf{P}_{T\alpha}(x) \cdot \mathbf{A}_T(x).
\]
(13)

It follows from Eqs. (11) and (12) that we may set
\[
\mathbf{P}_{T\alpha}(x) = -\int d^3x' \mathbf{g}_{T\alpha}(x, x') \rho(x')
\]
\[
= \alpha q \int_0^1 d\lambda \mathbf{r} \cdot \delta^T(x - \lambda \mathbf{r}) = \alpha \mathbf{P}_T(x),
\]
(14)  \\
where \( \mathbf{P}_T := \mathbf{P}_{T1} \) is the multipolar transverse polarisation. According to these definitions, in the Coulomb gauge we have \( \mathbf{P}_{T0} = 0 \) and therefore \( \mathbf{P}_0 = \mathbf{P}_L \). In the multipolar-gauge we have
\[
\mathbf{P}_1(x) := \mathbf{P}_{T1} + \mathbf{P}_L = q \int_0^1 d\lambda \mathbf{r} \delta(x - \lambda \mathbf{r}).
\]
(15)

This field specifies a straight line of singular dipole moment density, that stretches from the charge \(-q\) at \( \mathbf{0} \) to the dynamical charge \( q \) at \( \mathbf{r} \).

We now provide a canonical (Hamiltonian) quantum description. Typically this would be derived from a suitable Lagrangian and the gauge would be fixed from the outset. However, our only requirement is that the theory produces the correct Maxwell-Lorentz system of equations and it can therefore be obtained through a series of ansatzes. A rigorous and more general derivation of arbitrary-gauge QED is given using modern gauge-field theory in Secs. II B-II D.

We proceed by writing down the total energy of the system as the sum of kinetic and electromagnetic energies;
\[
E = \frac{1}{2m} \mathbf{p}^2 + \frac{1}{2} \int d^3x (\mathbf{E}^2 + \mathbf{B}^2)
\]
\[
= \frac{1}{2} m \dot{\mathbf{r}}^2 + U(\mathbf{r}) + V_{\text{self}}(\mathbf{r}) + \frac{1}{2} \int d^3x (\mathbf{E}_T^2 + \mathbf{B}^2),
\]
(16)  \\
where \( \mathbf{E}_T = -\dot{\mathbf{A}}_T \) and
\[
U(\mathbf{r}) + V_{\text{self}} = \frac{1}{2} \int d^3x \mathbf{E}_L^2 = \frac{1}{2} \int d^3x \mathbf{P}_L^2.
\]
(17)

Here \( U(\mathbf{r}) = -q^2/(4\pi|\mathbf{r}|) \) is the Coulomb energy binding the charges \( q \) and \(-q \) and \( V_{\text{self}} \) is the sum of the infinite Coulomb self-energies of each individual charge. Eq. (17) is obtained by solving Gauss’ law \( \nabla \cdot \mathbf{E} = \rho \), which yields \( \mathbf{E}_L = -\mathbf{P}_L = -\nabla \phi \) with \( \phi \) defined in Eq. (8).

We now assume that the canonical operators \( \mathbf{y} = \{ \mathbf{r}, \mathbf{A}_T, \mathbf{p}, \Pi \} \) in terms of which we will express the theory, satisfy
\[
[r_i, p_j] = i\delta_{ij},
\]
(18)
\[
[A_{T,i}(x), \Pi_{T,j}(x')] = i\delta^{ij}(x - x').
\]
(19)

All other commutators between canonical operators are assumed to vanish.

Since energy generates translations in time, the Hamiltonian that we seek must equal the total energy expressed in terms of the canonical operators; \( H(\mathbf{y}) = E \). Given this constraint we must now make suitable ansatzes for the velocities \( \dot{\mathbf{r}} \equiv \dot{\mathbf{r}}(\mathbf{y}) \) and \( \dot{\mathbf{A}}_T \equiv \dot{\mathbf{A}}_T(\mathbf{y}) \). We require that upon substitution into the right-hand-side of Eq. (16) our ansatzes define a Hamiltonian \( H(\mathbf{y}) \), which yields the correct Maxwell-Lorentz equations when using the Heisenberg equation \( \dot{O} = -i[O, H] \) together with Eqs. (18) and (19).

Since we wish to provide a Hamiltonian description in an arbitrary gauge we make the arbitrary-gauge minimal-coupling ansatzes
\[
m\dot{\mathbf{r}} = \mathbf{p} - q\mathbf{A}_\alpha(\mathbf{r}),
\]
(20)
\[
\dot{\mathbf{A}}_T = \Pi + \mathbf{P}_{T\alpha}.
\]
(21)

From Eqs. (16), (20), and (21) we then obtain
\[
E = \frac{1}{2m} [\mathbf{p} - q\mathbf{A}_\alpha(\mathbf{r})]^2 + U(\mathbf{r}) + V_{\text{self}}
\]
\[
+ \frac{1}{2} \int d^3x \left( (\Pi^2 + \mathbf{P}_{T\alpha}^2) + (\nabla \times \mathbf{A}_T)^2 \right) =: H_\alpha(\mathbf{y}).
\]
(22)

This defines the arbitrary gauge Hamiltonian \( H_\alpha \), which coincides with the one derived in Refs. [4–6]. The CCR algebra giving Eqs. (18) and (19) provides an algebraic representation of differentiation, implying that
\[
\mathbf{p} - q\mathbf{A}_\alpha(\mathbf{r}) = -im [\mathbf{r}, H_\alpha],
\]
(23)
\[
\Pi(\mathbf{x}) + \mathbf{P}_{T\alpha}(\mathbf{x}) = -i[\mathbf{A}_T(\mathbf{x}), H_\alpha].
\]
(24)

This shows that the ansatzes in Eqs. (20) and (21) are self-consistent, because they are re-obtained using the Heisenberg equation. It is a straightforward exercise to verify that \( H_\alpha \) does indeed yield the correct Maxwell-Lorentz system of equations for any choice of gauge \( \alpha \).

It is readily verified that Hamiltonians of different fixed gauges \( \alpha \) and \( \alpha' \) are unitarily equivalent;
\[
H_{\alpha'} = R_{\alpha\alpha'} H_\alpha R^\dagger_{\alpha\alpha'},
\]
(25)
where \( R_{\alpha\alpha'} \) is called a gauge-fixing transformation and is defined by [4, 6, 31, 37, 38]
\[
R_{\alpha\alpha'} := \exp \left( i \int d^3x [\mathbf{P}_{T\alpha}(\mathbf{x}) - \mathbf{P}_{T\alpha'}(\mathbf{x})] \cdot \mathbf{A}_T(\mathbf{x}) \right)
\]
\[
= \exp (-iq[\chi_\alpha(\mathbf{r}) - \chi_{\alpha'}(\mathbf{r})])
\]
(26)
in which the second equality follows from Eq. (13). We emphasise that the definition of gauge-freedom continues to be the freedom to choose α, which specifies $A_L$. It therefore constitutes the freedom to transform between distinct minimal-coupling prescriptions within the Hamiltonian;

\[
\begin{align*}
R_{\alpha\alpha'} [p - qA_\alpha (r)] R_{\alpha\alpha'}^{-1} & = p - qA_{\alpha'} (r) \quad (27) \\
R_{\alpha\alpha'} (\Pi + P_{T_\alpha}) R_{\alpha\alpha'}^{-1} & = \Pi + P_{T_{\alpha'}} \quad (28)
\end{align*}
\]

Eq. (25) follows from these equations. The effect of the transformation has been the replacement \((A_\alpha, P_{T_\alpha}) \rightarrow (A_{\alpha'}, P_{T_{\alpha'}})\), which clearly constitutes a gauge-transformation from the fixed gauge α to the fixed gauge α'. The reason Eq. (28) occurs is that in Eq. (9) we chose to fix the gauge $A_L$ as a functional of $A_T$, which generates translations in $\Pi$. The gauge-freedom already inherent in the polarisation field is discussed further in Appendix VI.

We remark that in order to implement the gauge transformation $p - qA(r) \rightarrow p - qA(r) + \nabla\chi(r)$ the canonical momentum must transform as $e^{iq\chi(r)}pe^{-iq\chi(r)} = p - q\nabla\chi(r)$, which states that $r$ represents translations in $p$. This property relies upon the canonical commutation relation in Eq. (18). Eq. (27) in particular, features the gauge-fixing transformation $R_{\alpha\alpha'} = e^{-iq\chi_\alpha(r) - x_{\alpha'}(r)}$, the CCR algebra cannot be supported by a finite-dimensional Hilbert space. Thus, retaining only a finite number of material energy levels will ruin gauge-invariance. Material truncation is discussed in detail in Sec. III.

B. The gauge-principle and gauge-freedom

We now provide a rigorous derivation of arbitrary gauge non-relativistic QED using the principles of modern gauge-field theory. Our purpose is to show that the implications of gauge-freedom that will be discussed in Secs. III onward are a fundamental feature of QED, and not in any way an artefact of approximations or simplifications. This derivation also shows that gauge-freedom is much more general than the one-parameter freedom introduced above. The reader more interested in applications and implications of the arbitrary-gauge formalism may proceed directly to Sec. III.

We derive the theory of an atom within the quantised electromagnetic field. The Lagrangian is defined over Minkowski spacetime $E^{1,3}$. With respect to the atomic rest frame a vector $v \in E^{1,3}$ has components $v^0 = (\eta_0, v)$. We assume a non-relativistic (Schrödinger) matter-field $\psi$ with charge $q$ and without spin. The formalism is easily extended to include spin and is equally applicable to the relativistic Dirac-field [31]. The four-current $j$ has components $j^\mu = (\rho, J)$ where $\rho = q\psi^\dagger \psi$ and $J = -ie(\psi^\dagger \nabla \psi - (\nabla \psi^\dagger) \psi)/2m$ with $m$ the electronic mass.

Let $\mathcal{G}$ be a (Lie) group called the gauge group and let $g: E^{1,3} \rightarrow \mathcal{G}$. The gauge-principle asserts that:

- The form of electromagnetic and other interactions should be invariant under the local action of $\mathcal{G}$ on the matter field $\psi$, written $\psi'(x) = g(x) \cdot \psi(x)$. In QED $\mathcal{G} = U(1)$ and $\psi'(x) = e^{iq\chi(x)} \psi(x)$ where $\chi$ is arbitrary.

The definition of group action is textbook group theory [39]. In electrodynamics the above requirement is fulfilled if the matter-field interacts with a gauge-field via the replacement $-i\partial_\mu \rightarrow -i\partial_\mu + qA_\mu$ made for each $\mu$ within the material Lagrangian. Here $A_\mu = (A_0, -A)$ are the components of the gauge-potential $A$ and any two potentials $A$ and $A'$ such that

\[
A'(x) = g(x)A(x)g(x)^{-1} - g(x)dg(x)^{-1} = A(x) - d\chi(x)
\]

are physically equivalent, where $d$ denotes the exterior derivative [40, 41].

Mathematically, the classical field $\psi : E^{1,3} \rightarrow \mathbb{C}$ is a section of the trivial bundle $E = E^{1,3} \times \mathbb{C}$ and the phases $e^{iq\chi(x)}$ are identifiable as transition maps on the intersections of open regions in $E^{1,3}$ meaning that the gauge group $\mathcal{G}$ is the structure group of the bundle [40, 41]. The gauge-potential $A$ is an $E^{1,3}$-valued connection one-form mapping from the tangent bundle $TE^{1,3}$ [41]. The potentials $A$ and $A'$ are said to be related by a gauge-symmetry transformation. The spatial replacement $-i\nabla \rightarrow -i\nabla - qA$ is called the minimal-coupling replacement and the gauge-principle asserts that within this replacement the longitudinal potential $A_0$ can be freely chosen. In this sense $A_L$ is superfluous, i.e., redundant. A choice of $A_L$ fixes the gauge.

A suitable Lagrangian-density is [24]

\[
\mathcal{L} = \frac{i}{2} \left( \psi^\dagger \dot{\psi} - \psi^\dagger \gamma^0 \psi \right) - U + qA_0\psi^\dagger \psi + \frac{1}{2} (E^2 - B^2) - \frac{1}{2m} \left( ( -i\nabla - qA) \psi^\dagger \right) \cdot \left( ( -i\nabla - qA) \psi \right) \tag{30}
\]

where $U$ is an external potential due for example to nuclei, and where $E$ and $B$ are the electric and magnetic fields. The Lagrangian is degenerate due to gauge-redundancy, which is implied by the occurrence of non-dynamical constraints $\{C\}$ [42, 43]. The Hamiltonian description must therefore be obtained by Dirac’s method [42]. The naive Hamiltonian acts within a space $\mathcal{H}$ containing the physical state space $\mathcal{H}_p$ as a proper subspace comprised of vectors $|\psi\rangle$ such that $C|\psi\rangle = 0$. The momentum $\Pi_0$ conjugate to $A_0$ vanishes identically, while the momentum conjugate to $A$ is $\Pi \equiv -E$, where $E = E_T + E_L$ is the total electric field.

Altogether there are three constraints, which are $\{\Pi_0, \rho + v^\dagger \Pi, F(A)\}$ where $F(A)$ is a gauge-fixing constraint. The naive equal-time canonical brackets are [38, 42–44]

\[
\{\psi(x), \psi^\dagger(x')\} = \delta(x - x'), \quad [A_\mu(x), \Pi_\nu(x')] = i\delta_{\mu\nu}\delta(x - x').
\]

\[
\{\psi(x), \psi^\dagger(x')\} = \delta(x - x'), \quad [A_\mu(x), \Pi_\nu(x')] = i\delta_{\mu\nu}\delta(x - x').
\]

\[
\{\psi(x), \psi^\dagger(x')\} = \delta(x - x'), \quad [A_\mu(x), \Pi_\nu(x')] = i\delta_{\mu\nu}\delta(x - x').
\]
The first-class constraints $\Pi_0$ and $G = \nabla \cdot \mathbf{A} + \rho$ generate transformations between the redundant degrees of freedom. More specifically, the infinitesimal generator $\mathcal{G}[\chi]$ of a $U(1)$ gauge-symmetry transformation $S_\chi = e^{-i\mathcal{G}[\chi]}$ is given by

$$\mathcal{G}[\chi] = \int d^3x \left[ \Pi_0 \dot{\chi} + (\nabla \cdot \mathbf{A} + \rho) \chi \right].$$

(33)

As is easily verified using Eqs. (31) and (32), $S_\chi$ transforms the matter-field as

$$S_\chi \psi(x) S_\chi^\dagger = e^{i\xi(x)} \psi(x)$$

(34)

and the gauge-potential as

$$S_\chi A(x) S_\chi^\dagger = A(x) - d\chi(x).$$

(35)

According to the naive Hamiltonian defined using $\mathcal{L}$ the scalar potential acts as a Lagrange multiplier [43]. The time evolution of $A_0$ is completely arbitrary and is restricted to the non-physical subspace, so $A_0$ can be removed immediately. The constrained degrees of freedom $A_1$, and $A_0$ will later be seen to emerge in terms of gauge-invariant quantities within the final unconstrained theory. The Hamiltonian-density is now given by

$$\mathcal{H}' = \frac{1}{2m} \left[ (i\nabla - q \mathbf{A}) \psi^\dagger \right] \cdot \left[ (i\nabla - q \mathbf{A}) \psi + \psi^\dagger \mathbf{U} \psi \right]$$

$$+ \frac{1}{2} \left[ \mathbf{P}^2 + (\nabla \times \mathbf{A})^2 \right]$$

(36)

and gauge-symmetry transformations are given by [37]

$$S_\chi = \exp \left[ -i \int d^3x \, G \chi \right].$$

(37)

Since $G$ commutes with the Hamiltonian the subspace defined by $G$ is dynamically invariant. The naive theory does not yield the correct Maxwell-Schrödinger system of equations, because the remaining constraints have not yet been imposed. The procedure for obtaining the correct unconstrained theory is now given.

A realization of the algebra of the canonical Maxwell operators $\mathbf{A}$ and $\mathbf{P}$ is given on $\mathcal{H}$ using the representations

$$(\hat{A}_\phi)[\mathbf{A}] = \mathbf{A} \phi[\mathbf{A}], \quad (\hat{P}_\phi)[\mathbf{A}] = -i \frac{\delta \phi[\mathbf{A}]}{\delta \mathbf{A}}$$

(38)

where $\phi$ is a wave-functional of $\mathbf{A}$ and where we have introduced hats to distinguish between operators and classical vector fields. Letting $\mathbf{A}_L = \nabla \chi$, we can vary the wave functional $\phi$ with respect to $\chi$ and make use of Eq. (38) to obtain

$$i \frac{\delta \phi}{\delta \chi} = -i \nabla \cdot \delta \phi = -i \nabla \cdot \frac{\delta \phi}{\delta \mathbf{A}_L} = \nabla \cdot \hat{\mathbf{A}}_L \phi = \nabla \cdot \hat{\mathbf{P}} \phi.$$  

(39)

Using the constraint $G$ a physical state $\varphi_p$ is therefore seen to be such that

$$i \frac{\delta \varphi_p}{\delta \chi} = -\rho \varphi_p.$$  

(40)

Solving this equation gives the general form of a physical state $\varphi_p$ [31, 37, 38]:

$$\varphi_p[\mathbf{A}] = \exp \left( i \int d^3x \chi(x) \rho(x) \right) \varphi_p[\mathbf{A}_T].$$  

(41)

We note that in a similar fashion, had we initially employed the representation $\Pi_0 = -i\delta / \delta A_0$ we would have immediately found that $\varphi_p$ does not depend on $A_0$ by solving the equation $\Pi_0 \varphi_p = 0$ [38].

In Ref. [37] a unitary gauge-fixing transformation yielding the Coulomb-gauge theory is given as

$$U \equiv \exp \left( -i \int d^3x \chi(x) \rho(x) \right)$$

(42)

where $(\chi \varphi)[\mathbf{A}] = \chi \varphi[\mathbf{A}]$ for all $\varphi[\mathbf{A}]$. In the present context we see clearly that $U$ eliminates the dependence of the physical state on $\mathbf{A}_L$:

$$(U \varphi_p)[\mathbf{A}] = \varphi_p[\mathbf{A}_T].$$

(43)

This corresponds to choosing the constraint $\mathcal{F}(\mathbf{A}_L) = \mathbf{A}_L$ for which the physical subspace is such that $\mathbf{A}_L \phi = 0$. More generally, we can use the transverse vector potential to specify any other vector potential [31, 38]. This results from employing the gauge-fixing constraint $\mathcal{F}(\mathbf{A}_L) = \mathbf{A}_L(x) - \nabla \chi_g(x, \mathbf{A}_T)$ such that on the physical subspace:

$$\mathbf{A}_L = \nabla \chi_g(x, \mathbf{A}_T)$$

(44)

where we could, for example, follow Ref. [44] by setting

$$\chi_g(x, \mathbf{A}_T) = \int d^3x' g(x', x) \cdot \mathbf{A}_T(x').$$

(45)

in which $g$ is the green’s function for the divergence operator; $\nabla \cdot g(x, x') = \delta(x - x')$. The gauge is now set by a choice of transverse green’s function, which beyond a requirement of sensible mathematical behaviour, is completely arbitrary, but is also non-dynamical and classical. We refer to a specific choice of $g_{GT}$ as selecting the gauge $g$. The above form of gauge-function $\chi_g$ is sufficiently general to yield the standard Coulomb and multipolar-gauge descriptions of non-relativistic QED as special cases [44].

A general unitary gauge-fixing transformation $U_g$ is defined by [31, 37]

$$U_g := \exp \left( -i \int d^3x \left[ \hat{\chi}(x) - \chi_g(x, \hat{\mathbf{A}}_T) \right] \rho(x) \right).$$

(46)

The physical subspace can be realised as any of the isomorphic spaces $\mathcal{H}_g = \{ |\psi\rangle \in U_g \mathcal{H} : U_g \mathcal{G} U_g^\dagger |\psi\rangle = 0 \}$
labelled by the gauge \( g \). Evidently \( \mathcal{H}_g \) is dynamically invariant. A generic element of \( \mathcal{H}_g \) is

\[
(U_g \varphi_p)[A] = \exp \left( i \int d^3x \varphi_g(x, A_T)p(x) \right) \varphi_p[A_T]
\]

\[
= \varphi_p[A_T + \nabla \chi_g] =: \varphi_g[A_T] \in \mathcal{H}_g.
\]  

(47)

The vector potential operator in the gauge \( g \) is defined by \( \mathbf{A}_g(x) := \mathbf{A}_T(x) + \nabla \chi_g(x, \mathbf{A}_T) \) such that

\[
(\hat{\mathbf{A}}_g \varphi_g)[A_T] = (A_T + \nabla \chi_g)\varphi_g[A_T].
\]

(48)

The unitary transformation from the fixed gauge \( g \) to the fixed gauge \( g' \) is

\[
U_{gg'} := \exp \left( -i \int d^3x \left[ \chi_g(x, \mathbf{A}_T) - \chi_g'(x, \mathbf{A}_T) \right] \rho(x) \right),
\]

(49)

an example of which is the well-known Power-Zienau-Woolley transformation. These transformations are clearly distinct from the gauge-symmetry transformations \( S_\chi \) of the original (constrained) theory in that they do not directly transform \( \mathbf{A}_g \), with which they commute. It is therefore evident that within Hamiltonian QED the single label “gauge transformation” is semantically inadequate, because transforming to a new gauge requires us to use different mathematical generators depending on the stage of development of the theory. Before any constraints are imposed a gauge-symmetry transformation \( S_\chi \) is required whereas in the final unconstrained theory a gauge-fixing transformation \( U_{gg'} \) is required. The significance of this distinction is discussed in further detail in Sec. III.

C. Hamiltonian in gauge \( g \)

To obtain the Hamiltonian in the gauge \( g \) we simply need to determine the effect of \( U_g \) on the remaining operators of the theory, namely \( \psi \), \( \bar{\psi} \) and \( \Pi \). In so doing we will resume denoting operators without hats. To find the transformation of \( \Pi \) it is convenient to define the polarisation field \( \mathbf{P}_g \) such that \( -\nabla \cdot \mathbf{P}_g = \rho \) [see also Appendix VI]. The longitudinal part of \( \mathbf{P}_g \) is unique being given by \( \mathbf{P}_L = \nabla \phi \) where \( \phi \) is defined in Eq. (8), whereas the transverse part \( \mathbf{P}_{Tg} \) is completely arbitrary and is defined by

\[
\mathbf{P}_{Tg}(x) = -\int d^3x' \frac{\Delta \chi_g(x', [A_T])}{\delta A_T(x)} \rho(x').
\]

(50)

In particular, choosing \( \chi_g \) as in Eq. (45) gives

\[
\mathbf{P}_g(x) = -\int d^3x' \mathbf{g}(x, x') \rho(x').
\]

(51)

where \( \mathbf{g} = \mathbf{g}_L + \mathbf{g}_T \) with \( \mathbf{g}_L(x, x') = -\nabla (1/4 \pi |x - x'|) \) and \( \mathbf{g}_T(x, x') \) arbitrary. Using \( \Pi = -i\delta/\delta \mathbf{A} = -i\delta/\delta \mathbf{A}_T - i\delta/\delta \mathbf{A}_L \) it is easily verified that for \( U_g \) defined in Eq. (46), we have

\[
U_g \Pi \Pi^+_g = \Pi + \mathbf{P}_g
\]

(52)

where \( \mathbf{P}_g = \mathbf{P}_L + \mathbf{P}_{Tg} \) with \( \mathbf{P}_{Tg} \) defined by Eq. (50). The constraint \( G \) and the residual gauge transformation \( S_\chi \) therefore transform as;

\[
U_g G \Pi^+_g = \nabla \cdot \mathbf{P},
\]

(53)

\[
U_g S_\chi \Pi^+_g = \exp \left( i \int d^3x \mathbf{P} \cdot \nabla \right),
\]

(54)

which are both independent of \( g \). The constraint \( U_g G \Pi^+_g |\psi\rangle = 0 \) implies that the longitudinal canonical momentum \( \Pi_L \) vanishes on \( \mathcal{H}_g \), i.e., that \( \Pi = \Pi_T \) such that \( \Pi \) admits the representation \( \Pi = -i\delta/\delta \mathbf{A}_T \). It also follows that \( S_\chi \) is the identity on \( \mathcal{H}_g \). Thus, all gauge-redundancy within the state space has been eliminated.

Before transformation by \( U_g \) the operator \( \Pi \) represented the field \( -\mathbf{E} \), which implies that in the gauge \( g \) the operator \( U_g \Pi \Pi^+_g = \Pi + \mathbf{P}_g \) represents \( -\mathbf{E} \). Since on \( \mathcal{H}_g \) we have \( \Pi = \Pi_T \), it follows that

- In the gauge \( g \) the operator \( \Pi \) represents the field \( -\mathbf{E} - \mathbf{P}_g = -\mathbf{E}_T - \mathbf{P}_{Tg} \).

We will see that in applications this is an especially important feature of the theory. Hereafter we use subscripts to denote contravariant indices. On \( \mathcal{H}_g \) the commutator of the transverse operators \( \mathbf{A}_T \) and \( \Pi \) follows from the naive commutator in Eq. (32), and is found to be

\[
[A_T, i(x)\Pi_j(x')] = \int d^3y d^3z \delta_{ijk} \delta^T_{ji} \left[ A_k(y), -i \frac{\delta}{\delta A_j(z)} \right] = i\delta^T_{ij}(x - x')
\]

(55)

where we have used the transversality of \( \mathbf{A}_T \) and the transversality of \( \Pi \) on \( \mathcal{H}_g \). Finally, the transformation of \( \psi \) by \( U_g \) is easily found to be

\[
U_g \psi \Pi^+_g = e^{i g(x - x_0) \psi}.
\]

(56)

Like \( \Pi \) the fermionic operator \( \psi \) is implicitly different in each gauge \( g \).

Having determined all operators in the gauge \( g \) we can now write the Hamiltonian density \( \mathcal{H} \) in the gauge \( g \) as

\[
\mathcal{H}_g = \frac{1}{2m} \left[ (i\nabla - q \mathbf{A}_g) \psi^\dagger \right] \left[ (i\nabla - q \mathbf{A}_g) \psi \right] + |\psi^\dagger U \psi|^2 + \frac{1}{2} \left[ (\Pi + \mathbf{P}_g)^2 + (\nabla \times \mathbf{A}_g)^2 \right] = U_g \mathcal{H} U_g^\dagger
\]

(57)

where we have adopted a normal-ordering of the final term and it is understood that \( \mathcal{H}_g \) is defined over \( \mathcal{H}_g \). Both the longitudinal part of \( \mathbf{A}_g \) and the transverse part of \( \mathbf{P}_g \) are arbitrary. Within the Hamiltonian a gauge
transformation of either one of these quantities using \( U_{gg'} \) necessarily incurs an accompanying gauge transformation of the other. The transformations are implemented via the canonical momenta \( \psi^\dagger(-i\nabla)\psi \) and \( \Pi \) as

\[
U_{gg'}\psi^\dagger(-i\nabla - qA_g)\psi U_{gg'}^\dagger = \psi^\dagger(-i\nabla - qA_{g'})\psi, \tag{58}
\]
\[
U_{gg'}(\Pi + \mathbf{P}_{Tg})U_{gg'}^\dagger = \Pi + \mathbf{P}_{Tg'}, \tag{59}
\]

which generalise Eqs. (27) and (28) respectively. The Hamiltonians of different gauges are related by

\[
H_g = U_{gg'}^\dagger H_{g'} U_{gg'} \tag{60}
\]

The Hamiltonian \( H_g \) can be partitioned in a number of illuminating ways. Noting that \(-i\nabla - qA_g \) is the single-particle mechanical momentum operator, the first term on the top line of Eq. (57) is the material kinetic energy-density \( \delta_{KE} \), while the second term \( \delta_U := \psi^\dagger U\psi \) is the potential energy-density due to the external potential \( U \). Since on \( H_g \) we have \( E = -\Pi - \mathbf{P}_g \), the term on the second line in Eq. (57) is the electromagnetic energy-density \( \delta_{EM} := (\mathbf{E}^2 + \mathbf{B}^2)/2 \). The Hamiltonian therefore represents the total energy in any gauge \([31]\);

\[
H_g = E = E_{KE} + E_U + E_{EM}. \tag{61}
\]

Furthermore, on the space \( H_g \) we have \( \Pi = -E - \mathbf{P}_g \) and \( \Pi_L = 0 \), so the longitudinal field \( \mathbf{E}_L = -\mathbf{P}_L \) is uniquely specified as a function of \( \rho \). Thus, the electromagnetic energy \( E_{EM} \) can be partitioned into transverse and Coulomb components as

\[
E_{EM} = V_{Coul} + E_{TEM} \tag{62}
\]

where \( V_{Coul} = \int d^3x : \mathbf{E}_L^2 : /2 \) is the Coulomb energy-density, which we have assumed is normally-ordered, and where \( \delta_{TEM} := (\mathbf{E}^2 + \mathbf{B}^2)/2 \).

D. Re-emergence of the scalar potential

Since we have now fixed \( \mathbf{A}_L = \nabla \chi_g \) and we have also identified that the electric field is \( \mathbf{E} = -\Pi - \mathbf{P}_g \) we can identify, up to a constant, the scalar potential \( \phi_g \) within the gauge \( g \) from its fundamental definition \( \nabla \phi_g = -\mathbf{E} - \mathbf{A}_g \). We use this equality and the definition of \( \mathbf{A}_g \) together with \( \mathbf{E} = -\Pi - \mathbf{P}_g \) and \( \Pi_L = -\mathbf{E}_L = \nabla \phi \) where \( \phi \) is the Coulomb-gauge scalar potential (Coulomb potential) given in Eq. (8), to obtain

\[
\nabla \phi_g = \nabla(\phi - \partial_t \chi_g) - \mathbf{A}_T + \Pi + \mathbf{P}_{Tg}. \tag{63}
\]

Thus, we see that \( \phi_g \) is fully determined in terms of the transverse canonical operators and the matter field. Moreover, from the Hamiltonian \( H_g \) we easily find that

\[
\mathbf{A}_T = -i[\mathbf{A}_T, H_g] = \Pi + \mathbf{P}_{Tg} = -\mathbf{E}_T \tag{64}
\]

as expected, and using this result together with Eq. (63) we find that up to a constant

\[
\dot{\phi}_g = \phi - \partial_t \chi_g, \tag{65}
\]

which is the expected result for the scalar potential corresponding to the vector potential \( \mathbf{A}_g = \mathbf{A}_T + \nabla \chi_g \).

It is instructive to calculate in the arbitrary gauge \( g \), the equation of motion for the Schrödinger operator \( \psi \), which should be the Schrödinger equation in the presence of the Maxwell field and the external potential \( U \). A straightforward calculation yields the correct result

\[
i\dot{\psi} = [\psi, H_g] = \left[ \frac{1}{2m}(-i\nabla - qA_g)^2 + U + q\phi_g \right]\psi. \tag{66}
\]

Under the local phase transformation

\[
\psi \rightarrow e^{-iq(x', \chi_g)} \psi, \tag{67}
\]

the Schrödinger equation is unchanged in form but as required by the gauge-principle the potentials therein are replaced with the gauge-transformed potentials

\[
\phi_{g'} = \phi_g - \partial_t (\chi_g \cdot \chi_{g'}), \tag{68}
\]
\[
A_{g'} = A_g + \nabla (\chi_{g'} \cdot \chi_g). \tag{69}
\]

Eq. (66) reproduces as special cases the Schrödinger equations given by Power and Thirumalachandran in Ref. [45], which were derived from the Coulomb-gauge and multipolar-gauge Hamiltonians, but which were not expressed in terms of the corresponding potentials. We have shown that these Schrödinger equations are particular fixed-gauge cases of the expected general result that must be obtained according to the gauge principle, and that they are related by a gauge transformation.

E. Relation to the particle-based description

In the non-relativistic setting where matter is described by a Schrödinger field rather than a Dirac field there is no anti-matter, so the total material number operator is a conserved quantity \([24]\). One can therefore employ an equivalent description to the field-theoretic description derived above, whereby each electron is described using single-particle canonical position and momentum operators \( \mathbf{r} \) and \( \mathbf{p} \) such that \([r_i, p_j] = i\delta_{ij}\). For a given number of electrons the descriptions are strictly equivalent, but the particle-based description may be less cumbersome when dealing with simple systems.

The field density \( \rho = q\psi^\dagger \psi \) corresponds to the single-electron density \( q\delta(\mathbf{x} - \mathbf{r}) \). In Sec. II A we considered a single-electron atom with nucleus fixed at the origin such that the charge density is \( \rho(\mathbf{x}) = -q\delta(\mathbf{x}) + q\delta(\mathbf{x} - \mathbf{r}) \). The nuclear potential \( U(\mathbf{x})/q \) is therefore now included in the longitudinal electric field energy along with the infinite self-energies \( V_{self} = \int d^3x \mathbf{E}_L^2 \):

\[
\frac{1}{2} \int d^3x \mathbf{E}_L^2 \frac{1}{2} \int d^3x \mathbf{P}_L^2 = U(\mathbf{r}) + V_{self}. \tag{70}
\]
The transverse field $\mathbf{P}_T$ is unaffected. The Hamiltonian $H_g$ with density in Eq. (57) can now be written

$$H_g = \frac{1}{2m} [\mathbf{p} - q\mathbf{A}_g(\mathbf{r})]^2 + U(\mathbf{r}) + V_{\text{self}} + \frac{1}{2} \int d^3 x' \left[(\mathbf{\Pi} + \mathbf{P}_{Tg})^2 + (\nabla \times \mathbf{A}_T)^2\right]$$

(71)

where, assuming $\chi_g$ as in Eq. (45), we have

$$\mathbf{A}_g(\mathbf{x}) = \mathbf{A}_T(\mathbf{x}) + \nabla \int d^3 x' \mathbf{g}(\mathbf{x}', \mathbf{x}) \cdot \mathbf{A}_T(\mathbf{x}'),$$

(72)

$$\mathbf{P}_{Tg}(\mathbf{x}) = - \int d^3 x' \mathbf{g}_T(\mathbf{x}, \mathbf{x}') \rho(\mathbf{x}').$$

(73)

The theory is simplified further by restricting $\mathbf{g}_T$ via Eq. (12) in terms of the gauge-parameter $\alpha$. These simplifications are not approximations, so the theory remains exact and it becomes the theory presented in Sec. II A. Therein gauge-freedom is the freedom to choose the parameter $\alpha$ which specifies $\mathbf{P}_{T\alpha}$ and $\mathbf{A}_\alpha$ as in Eqs. (14) and (9) respectively [4–6]. The Hamiltonian $H_g$ in Eq. (71) becomes $H_\alpha$ given in Eq. (22) and the gauge-fixing transformation $U_{g\alpha'}$ in Eq. (49) becomes $R_{\alpha\alpha'}$ in Eq. (26). Hamiltonians belonging to different gauges are unitarily related as in Eq. (25).

**F. Electric dipole approximation**

The electric-dipole approximation (EDA) of the theory presented in Sec. II A can be performed preserving all kinematic and algebraic relations of the theory such that gauge-invariance is also preserved. Considering a dipole centred at the origin $0$ the EDA is defined by

$$\chi_\alpha(\mathbf{r}) \approx -\alpha \mathbf{r} \cdot \mathbf{A}_T(\mathbf{0}),$$

(74)

$$\mathbf{A}_\alpha(\mathbf{r}) \approx (1 - \alpha)\mathbf{A}_T(\mathbf{0}),$$

(75)

$$\mathbf{P}_{T\alpha,i}(\mathbf{x}) \approx \alpha q r_f \delta_{ij}(\mathbf{x}).$$

(76)

When these approximate equalities are substituted into Eq. (22) the $\alpha$-gauge Hamiltonian in EDA is obtained. Similarly, the unitary gauge-fixing transformation $R_{\alpha\alpha'}$ in Eq. (26) becomes

$$R_{\alpha\alpha'} = \exp \left[i(\alpha - \alpha')q \mathbf{r} \cdot \mathbf{A}_T(\mathbf{0})\right].$$

(77)

Since unitarity is preserved, so too is gauge-invariance [cf. Sec. II K]. Hamiltonians belonging to different gauges continue to be unitarily equivalent as in Eq. (25).

**G. Physical nature of the gauge-function $\mathbf{g}_T$**

Looking toward applications of the formalism so far developed, we now seek to understand the ways in which different fixed-gauge formulations of QED differ. The gauge is selected by choosing $\chi_g$. If $\chi_g$ is restricted in form as in Eq. (45) then the gauge is selected by choosing a concrete transverse function $\mathbf{g}_T$. The gauge choice directly specifies two basic quantities, $\mathbf{A}_g$ and $\mathbf{P}_{Tg}$. This in turn specifies the physical nature of the canonical momenta $\mathbf{p}$ and $\mathbf{\Pi}$, which together with $\mathbf{r}$ and $\mathbf{A}_T$ define the quantum subsystems conventionally termed “matter” and “light”. The importance of this fact is the main topic of the present article and will be described in detail in the remainder of this section (Secs. III H–III L).

To better understand the full scope of the gauge-freedom we first restrict our attention to gauges of the form in Eq. (45). It is convenient to introduce the unconstrained function $\mathbf{G}$, which is essentially completely arbitrary (not necessarily transverse in the first argument), such that

$$\tilde{\mathbf{g}}_T(\mathbf{k}, \mathbf{x}) = \sum_\alpha \mathbf{e}_\alpha(\mathbf{k}) [\mathbf{e}_\alpha(\mathbf{k}) \cdot \mathbf{G}(\mathbf{k}, \mathbf{x})]$$

(78)

where $\tilde{\mathbf{g}}_T$ denotes Fourier transforms and where $\mathbf{e}_\sigma(\mathbf{k})$, $\sigma = 1, 2$ are orthonormal vectors spanning the plane orthogonal to $\mathbf{k}$. It is instructive to consider how the present arbitrary-gauge formalism is related to existing fixed-gauge formulations of QED. We have already seen that the two most commonly chosen gauges of non-relativistic QED can be linearly interpolated between via a parameter $\alpha$. This amounts to restricting $\mathbf{G}$ as

$$\tilde{\mathbf{G}}_\alpha(\mathbf{k}, \mathbf{x}) = \alpha \tilde{\mathbf{G}}_1(\mathbf{k}, \mathbf{x}) = -\frac{\alpha \mathbf{x}}{\sqrt{(2\pi)^3}} \int_0^1 d\lambda e^{-i\mathbf{k} \cdot \mathbf{x}}$$

(79)

where now only the parameter $\alpha$ is freely choosable. The multipolar-gauge $\alpha = 1$ specifies a singular polarisation $\mathbf{P}_{T1}$, which is often regularised at small distances [24, 46, 47]. This is achieved through the introduction of a Lorentzian with frequency cut-off $k_M$ as

$$\tilde{\mathbf{G}}_{\alpha M}(\mathbf{k}, \mathbf{x}) = -\frac{\alpha \mathbf{x}}{\sqrt{(2\pi)^3}} \frac{k_M^2}{k^2 + k_M^2} \int_0^1 d\lambda e^{-i\mathbf{k} \cdot \mathbf{x}}.$$  

(80)

For $k_M$ finite the field $\mathbf{P}_{T\alpha}$ is no longer singular at $0$. If $\mathbf{P}_L$ is similarly regularised then for $\alpha = 1$ the ensuing total polarisation $\mathbf{P}_L$ is no longer point-localised, but exponentially localised instead. Our treatment shows that this regularisation of $\mathbf{P}_{T\alpha}$ actually constitutes a choice of gauge, that is, we now have a two-parameter gauge function uniquely specified by a gauge vector $(\alpha, k_M)$. Only for $\alpha = 0$ do we have $\mathbf{P}_{T\alpha} = 0$ and $\chi_\alpha = 0$, such that regularisation of $\mathbf{P}_L$ has no effect on the Hamiltonian. More generally, we may simply let

$$\tilde{\mathbf{G}}_{\{\alpha\}}(\mathbf{k}, \mathbf{x}) = -\frac{\alpha(\mathbf{k})^* \mathbf{x}}{\sqrt{(2\pi)^3}} \int_0^1 d\lambda e^{-i\mathbf{k} \cdot \mathbf{x}},$$

(81)
which from Eqs. (45) and (73) yields

\[
\chi_g(x) = \int d^3k \sum_{\sigma} \alpha(k)e_\sigma(k) \cdot \tilde{A}_T(k)e_\sigma(k) \cdot \tilde{G}_1(k,x)^*,
\]

(82)

\[
\tilde{P}_{Tg}(k)^* = - \int d^3x \sum_{\sigma} \alpha(k)e_\sigma(k)e_\sigma(k) \cdot \tilde{G}_1(k,x)^* \rho(x)
\]

(83)

where \( \tilde{G}_1 \) is given in Eq. (79). The field \( \chi_g \) depends on photonic degrees of freedom through \( \tilde{A}_T \) and couples to the material momentum \( p \) within the Hamiltonian, while the field \( \tilde{P}_{Tg} \) depends on the material degrees of freedom through \( \rho \) and couples to the photonic momentum \( \tilde{H} \) within the Hamiltonian. Thus, Eq. (81) enables broad control over the physical nature of the light-matter coupling, because while it is restricted in its \( x \)-dependence, \( \alpha(k) = \alpha(-k)^* \) is essentially arbitrary. As an example, we will see in Sec. V that the gauge \( \alpha(k) = \omega_m/(\omega + \omega_m) \) where \( \omega_m \) is a material frequency, is noteworthy. It can be interpreted as defining a canonical harmonic dipole that automatically subsamples the virtual photons dressing the system ground state [4, 14, 15]. It is clear that \( g_T \) may be yet more general than those above and furthermore, the gauge function \( \chi_g \) need not even be restricted as in Eq. (45). This broad generality warrants further study, but will not be considered here.

H. Sharing out the constrained degrees of freedom: Regularisation and localisation

The choice of \( G \) determines the physical meaning of the canonical degrees of freedom. To see how, we will focus on the simple choices given by Eqs. (79) and (80). Let us first consider the simple “unregularised” one-parameter gauges whereby \( G_\alpha \) is defined by Eq. (79). First we consider the vector potential \( A_\alpha \) and the momentum \( p \) determined physically by \( A_\alpha \). According to Eq. (9) \( A_\alpha \) is a function of \( A_0 = A_T = (\nabla \times)^{-1} B \), so it can be expressed as a convex sum of the extremal potentials \( A_0 \) and \( A_1 \):

\[
A_\alpha(x) = (1 - \alpha)A_0(x) + \alpha A_1(x) = \int d^3x' \frac{(1 - \alpha)\nabla' \times B(x')} {4\pi |x - x'|} - \alpha \int_0^1 d\lambda \lambda x \times B(\lambda x).
\]

(84)

Eq. (84) shows that the potential \( A_\alpha(r) \), as appears in the Hamiltonian, is non-local in any gauge, but it is most localised in the multipolar-gauge, \( \alpha = 1 \), because all points \( x \) for which \( A_1(r) \) depends on the local field \( B(x) \) are inside the atom; \( |x| \leq |r| \). More precisely, \( A_1(r) \) depends on \( B \) only at points on the straight line connecting \( 0 \) to \( r \). The value of \( \alpha \) within the vector potential \( A_\alpha \), dictates the balance between this local contribution and the non-local contribution \( (1 - \alpha)A_0 \) given by the \( x' \) integral in Eq. (84).

To see most clearly how \( A_\alpha \) determines the physical nature of \( p \), which defines the canonical atom, we make the EDA

\[
\tilde{G}_\alpha(k,r) \approx \frac{\alpha r} {\sqrt{(2\pi)^3}}.
\]

(85)

which implies

\[
A_\alpha(r) := A_T(r) - \alpha \nabla r \int_0^1 d\lambda r \cdot A_T(\lambda r)
\]

\[
\approx A_T(0) - \alpha \nabla r [r \cdot A_T(0)] = (1 - \alpha)A_T(0).
\]

(86)

The quantity \( A_T(0) \) appearing on the right-hand-side is \( 1/|q| \) times the EDA of the momentum associated with the longitudinal electric field of the charge \( q \) at \( r \), viz. [24]

\[
K_{\text{long}} := \int d^3x E_{\text{lr}} \times B = qA_T(r)
\]

(87)

where \( E_{\text{lr}}(x) := -q\nabla(4\pi|x - r|)^{-1} \), consistent with Eq. (84). According to Eq. (86), the multipolar vector potential at the position of the dipole, \( A_1(0) \), vanishes at dipole order. The dipole canonical momentum is defined by \( p = m\dot{r} + qA_\alpha(0) \) where \( A_\alpha(0) = (1 - \alpha)A_T(0) \) [Eq. (86)]. For \( \alpha = 1 \) we have \( p = m\dot{r} \), such that \( E_l \) makes no contribution to the canonical pair \( \{r, p\} \), which is therefore “bare”. For \( \alpha = 0 \), the momentum \( p = m\dot{r} + K_{\text{long}} \) is fully dressed by \( E_{\text{lr}} \). Thus, the gauge \( \alpha \) controls the extent to which the canonical dipole is dressed by the electrostatic field of the dynamical charge \( q \) at \( r \).

Let us now repeat the above analysis in the case of the other quantity that is determined by the gauge \( \alpha \), namely \( P_{T\alpha} \). We will then see how this quantity determines the second canonical momentum \( \tilde{H} \). The total \( \alpha \)-gauge polarisation is \( P_\alpha = P_L + \alpha P_{T1} \), where \( P_L = -E_L \) is the non-local Coulomb-gauge polarisation and where \( P_{T1} \) is the transverse part of the multipolar polarisation. The total multipolar polarisation \( P_1 \) is given in Eq. (15), showing that it is a line integral that vanishes at all points \( x \) not on the straight line that connects \( 0 \) to \( r \). Therefore, outside the atom \( (|x| > |r|) \) we have \( P_{T1} = -P_L = E_L \). The \( \alpha \)-gauge polarisation can be written analogously to Eq. (84) as a convex sum of local and non-local extremal polarisations \( P_0 \) and \( P_1 \):

\[
P_\alpha = (1 - \alpha)P_0 + \alpha P_1.
\]

(88)

The polarisation \( P_0 \) is non-local in any gauge, but it is most localised in the multipolar-gauge, \( \alpha = 1 \), because all points \( x \) for which \( P_1(x) \neq 0 \) are inside the atom; \( |x| \leq |r| \). Within \( P_\alpha \), the value of \( \alpha \) dictates the balance between this local contribution and the non-local contribution \( (1 - \alpha)P_0 = -(1 - \alpha)E_L \).

As before, we can approximate the stationary atom as a dipole at the origin \( 0 \) using Eq. (85) to obtain \( P_1(x) = qr\delta(x) \) where \( qr \) is the dipole moment. Within
the fixed gauge \( \alpha \), the field canonical momentum operator is defined by \( \Pi = -E_T - \alpha P_{T1} = -E_T - \alpha E_L \) where the second equality holds for \( x \neq 0 \). Thus, the value of \( \alpha \) controls the extent to which the canonical pair \( \{ A_T, \Pi \} \), includes the electrostatic field \( E_L = E - E_T \). For \( \alpha = 0 \) we have \( \Pi = -E \) for \( x \neq 0 \), so the situation is reversed; \( E_L \) is fully included from the field canonical degrees of freedom. For \( \alpha = 1 \) we have \( \Pi = -E \) for \( x \neq 0 \), so the situation is reversed; \( E_L \) is fully included in the field canonical degrees of freedom for all \( x \neq 0 \).

Having determined both \( A_\alpha \) and \( P_{T\alpha} \) and both momenta \( p \) and \( \Pi \), we see clearly that the gauge \( \alpha \) controls the weight with which the field \( E_L \) is shared between the two canonical pairs \( \{ A_T, \Pi \} \) and \( \{ r, p \} \). For \( \alpha = 1 \) the static field is fully included in the field electrostatic subsystem and the dipole is “bare”. It should be noted that this is only true at dipole order. For \( \alpha = 0 \) the dipole is fully dressed by \( E_L \) and the field is purely transverse. This holds beyond the EDA, but the condition \( x \neq 0 \) must be replaced by \( |x| > |r| \) specifying all points outside the atom. The field \( E_L \) has been constrained by Gauss’ law which is what implied gauge-redundance; \( E_L \) is shared out differently for different choices of gauge \( \alpha \). This field lies at the heart of gauge-ambiguities in ultrastrong coupling QED. For example, the relation of electrostatic dressing to localisation and causality is discussed in the context of photodetection theory in Sec. IV.

We can also consider the regularisation of the above theory at short distances around the distribution centre \( 0 \) using \( G_{\alpha M} \) in Eq. (80), which within the EDA is

\[
\tilde{G}_{\alpha M}(k,r) \approx -\frac{\alpha r}{\sqrt{(2\pi)^3}} \frac{k^2_M}{k^2 + k^2_M}.
\]

The transverse \((\alpha,k_M)\)-gauge polarisation within the EDA is therefore

\[
P_{T\alpha M}(x) = \alpha q r \cdot \delta^T_M(x)
\]

where \( \delta^T_M(x) \) denotes the regularised transverse delta-function [24]

\[
\delta^T_M(x) = \frac{2}{3} \delta_{ij} \delta(x) - \frac{\beta(x)}{4\pi x^3} (\delta_{ij} - 3x_i \hat{x}_j),
\]

\[
\beta(x) = 1 - \left(1 + k_M x + \frac{1}{2} k^2_M x^2 \right) e^{-k_M x}.
\]

The function \( \beta(x) \) controls the singularity at \( 0 \), but is unity for \( x \gg 1/k_M \). The transverse delta-function \( \delta^T(x) \) is strictly recovered in the limit \( k_M \rightarrow \infty \). More generally, the previous \( \alpha \)-gauges constitute the \((\alpha, \infty)\) subset of the \((\alpha,k_M)\)-gauges. In the \((\alpha,k_M)\)-gauge the parameter \( \alpha \) functions as before while the additional gauge-parameter \( k_M \) controls the rate of exponential localisation of what was previously the singular point-like multipolar dipole. It is now the case that only for \( x \gg 1/k_M \) do we have \( P_{T}(x) = 0 \). Thus, there are now many “multipolar-gauges” specified by the gauge vectors \((1,k_M)\), each of which possesses a different degree of exponential dipolar localisation.

The \((\alpha,k_M)\)-vector potential is within the EDA

\[
A_{\alpha M}(r) \approx A_T(0) - \alpha \int d^3k \frac{k^2_M}{\sqrt{(2\pi)^3}} \frac{k^2_M}{k^2 + k^2_M} \tilde{A}_T(k),
\]

such that \( A_1(0) = 0 \) is recovered in the limit \( k_M \rightarrow \infty \). More generally, vanishing of \( A_{1M}(r) \) to dipole order requires that \( \tilde{A}_T(k) \approx 0 \) for \( k \geq k_M \). In order for this to be the case the modes \( k \geq k_M \) must not be populated. This is the case if the bare atom (as occurs in the free theory) is small compared to the characteristic wavelengths of the populated modes. In other words, the EDA places a lower bound on the cut-off \( k_M \). In order that \( \alpha = \alpha_M = 0 \) possess the property \( A_{1M}(0) = 0 \) that at dipole order parameterises the usual multipolar-gauge \((\alpha,k_M) = (1, \infty)\).

I. Discussion: Gauge-fixing, forms of rotation, forms of coupling, and common pitfalls

1. Gauge-freedom and gauge-fixing

We have defined the gauge principle according to modern gauge-field theory and we have given a formulation of canonical (Hamiltonian) non-relativistic QED in an arbitrary gauge. One of the main objectives of the present article is to clarify what gauge-freedom, gauge-fixing, and gauge-ambiguities are, within this theory:

- **Gauge-freedom** in electrodynamics is a freedom to choose \( A_L \). Once \( A_L \) is fixed then the corresponding scalar potential \( \phi_{A_L} \) is also fixed up to a constant by \( -\nabla \phi_{A_L} = E_L + A_L \). **Gauge-fixing** means specifying \( A_L \) in terms of gauge-invariant quantities.

We have provided a formulation of QED in which \( A_L \) is fixed by Eq. (44) as \( A_L(x) = -\nabla \chi_g(x, A_T) \) meaning it is fixed up to a choice of the non-operator-valued function \( g_T \). The corresponding vector and scalar potentials are given in accordance with their fundamental definitions by \( A_g = A_T + \nabla \chi_g \) and \( \phi_g = \phi - \partial_t \chi_g \) where \( E_L = -\nabla \phi \).

Confusion often arises in non-relativistic QED, due to claims that the multipolar field is preferable, because it can be expressed solely in terms of gauge-invariant electric and magnetic fields. However, the latter property holds in any gauge, by definition of gauge-fixing. We have already seen that the Hamiltonian always represents the total energy [Eqs. (61) and (16)] [4]. If one prefers to eliminate only \( A_\alpha \) from the expression for the Hamiltonian, but retain its explicit dependence on the canonical momenta, then this is easily achieved in any gauge \( \alpha \), using Eq. (84). Elimination of \( A_\alpha \) does not eliminate \( \Pi \) from the expression for the Hamiltonian. If one prefers to express the Hamiltonian in terms of electric and magnetic fields, but retain its dependence on \( p \), this is also
easily done, because \( \Pi = -E_T - P_{Ta} \). In particular, the Coulomb-gauge theory for which \( \Pi = -E_T \) can be expressed solely in terms of electric and magnetic fields, \( \mathbf{r} \) and \( \mathbf{p} \). The latter property is not unique to the multipolar theory.

2. Dipolar coupling

Another aspect of light-matter interactions, which is especially poorly understood, concerns the field that a dipole couples to within the multipolar-gauge. Common misidentifications are exacerbated by the development of textbooks that employ fully quantum descriptions. In previous textbooks (e.g. \[52\]) and more recently, in textbooks by Cohen-Tannoudji et al. \[24\]. From this point of view, any operator that does not commute with gauge-fixing transformations, such as \( \Pi \), will represent a different physical observable before and after such a transformation \[24\]. Conversely, any given physical observable will be represented by a different operator before and after transformation. For example, the energy \( E \) is represented by \( H_g(y) \) in gauge \( g \) and by \( H_g'(y) \) in gauge \( g' \). The eigenvalue equation \( H_g(y)|E_n^g\rangle = E_n^g|E_n^g\rangle \) implies that the vector \( |E_n^g\rangle \) represents, within the gauge \( g \), the physical state \( \mathcal{S}^g \) in which the system definitely possesses energy \( E_n^g \). Meanwhile, in the gauge \( g' \) the same state \( \mathcal{S}^g \) is represented by the different vector \( |E_n^{g'}\rangle = U_{gg'}|E_n^g\rangle \), because the energy is represented by the different operator \( H_{g'}(y) \).

Alternatively, a passive perspective of rotations may be adopted whereby different canonical operators are associated with different gauges as \( y_g = U_{gg'}y_{g'}U_{gg'}\). Notice that the rotation between canonical operators associated with different gauges \( g \) and \( g' \) is opposite to the rotation between the Hamiltonians associated with \( g \) and \( g' \) obtained via the active perspective. Nevertheless, the same relationship between Hamiltonian functions is obtained within the passive viewpoint by noting that \( H_g(y_g) = H_g(U_{gg'}y_{g'}U_{gg'}^\dagger) = U_{gg'}H_{g'}(y_{g'})U_{gg'}^\dagger = H_{g'}(y_{g'}) \). The passive perspective is also commonly found within the literature, for example, in the works of Power and Thirumalachandran \[28, 29, 45, 53-57\]. Therein, the Hamiltonian \( H_g(y_g) = H_{g'}(y_{g'}) \) is unique and it uniquely represents the energy \( E \). Similarly, the eigenvector \( |E_n^{g'}\rangle \) uniquely represents the physical state \( \mathcal{S}^{g'} \) of definite energy \( E_n^{g'} \). Conversely, each different set of canonical operators \( y_g \) represents a different set of physical observables. This again contrasts the active perspective wherein the physical difference between the same canonical operators \( y \) in different gauges was implicit.

Obviously, either an active or a passive perspective can be chosen, but the associations between operators and observables and between vectors and states will generally depend on the perspective adopted. The importance
of such associations and their relation to gauge-freedom is discussed in Secs. IIJ and IIK. Here, unless otherwise stated, we adopt an active perspective of unitary rotations.

4. Gauge-symmetry transformations versus gauge-fixing transformations

Confusion can stem from the fact that the PZW transformation \( R_{01} \) commutes with \( A_0 = \phi \) and \( A_0 = A_T \), so it cannot directly implement a gauge transformation as defined in Eqs. (68) and (69), as noted, for example, in Ref. [58]. However, it is clearly shown in Ref. [58] that the formulations of QED connected by \( R_{01} \) result from different choices of gauge. The situation becomes clear upon recognising that the PZW transformation is not a gauge-symmetry transformation \( S_X \), but a gauge-fixing transformation \( R_{01} \). The distinction between these types of gauge transformation has been known for a long time in relativistic physics [37], but is perhaps less well-known in quantum optics and atomic physics. Within the final unconstrained theory all gauge-symmetry transformations have been reduced to the identity, expressing the fact that once the gauge has been fixed there is no longer any redundancy within the state space or operator algebra. The redundant degrees of freedom \( A_1 \) have been fixed as known functions of the gauge-invariant degrees of freedom and the c-number \( g_T \). The gauge-fixing transformation \( U_{g'} \) transforms between alternative isomorphic realisations of the physical state space that result from different choices of the gauge \( A_1 = \nabla \chi_g \) and \( A_1 = \nabla \chi_{g'} \).

Although \( U_{g'} \) cannot transform \( (\phi, A_0) \) directly, it does so indirectly. To see this note that \( H_g(y) \) is shorthand for \( H(g_T, y) \) where the function \( H \) is unique. The concrete choice of function \( g_T \) used to evaluate \( H \) is left open. In other words, \( H_g(y) \) defined by \( H_g(y) := U_{g'} H_g(y) U_{g'}^\dagger \) is given by \( H_g(y) = H(g_T', y) \). By construction the functional form of the Hamiltonian in terms of \( g_T \), as well as all resulting dynamical equations written in terms of \( (\phi, A_0) \), are the same for every possible concrete choice of \( g_T \) (gauge). Thus, in the final unconstrained theory:

- Gauge-freedom is the freedom to transform between different Hamiltonians \( H_g \) and \( H_{g'} \) resulting from different fixed choices of the gauge \( g_T \) and \( g_T' \).

Formulations corresponding to different choices of \( g_T \) must be physically equivalent. The unitarity of gauge-fixing transformations \( U_{g'} \) ensures that this is the case, because the quantum-theoretic definition of physical equivalence is unitary equivalence (cf. Sec. IIJ).

5. Minimal-coupling

A final common pitfall that we wish to address concerns the nature of the minimal-coupling prescription and its relation to the Coulomb-gauge. In Sec. II A we saw that \( R_{\alpha \alpha'} \) implements a gauge change within the Hamiltonian by transforming between distinct minimal-coupling prescriptions [Eqs. (27) and (28)]. This shows that the minimal-coupling replacement is not synonymous with the Coulomb-gauge.

It is unfortunate that the term “minimal-coupling” has so often been reserved exclusively for the Coulomb-gauge Hamiltonian \( H_0 \), because this nomenclature is in direct opposition to the fundamental meaning of minimal-coupling. The gauge-principle implies the existence of a potential whose gauge \( A_L \) can be chosen freely. Different fixed gauges correspond to different fixed minimal-coupling replacements, as is clearly shown by Eqs. (22) and (27). This fact is obscured by the almost universal practice of expressing the multipolar potential \( A_1 \) in terms of \( B \) within the Hamiltonian via Eq. (84). It is then not obvious that the multipolar Hamiltonian does result from the minimal-coupling replacement \( p \rightarrow p - qA_1(r) \). Meanwhile, despite it being possible to express the Coulomb-gauge potential \( A_0 \) in terms of \( B \), the Coulomb-gauge Hamiltonian is nearly always left as a function of \( A_0 \). The minimal-coupling prescription \( p \rightarrow p - qA_0(r) \) is therefore immediately apparent therein. The combined effect of these conventions may be the false impression that only the Coulomb-gauge Hamiltonian results from minimal-coupling replacement. In fact, in any gauge \( \alpha \), the Hamiltonian includes a minimal-coupling replacement \( p \rightarrow p - qA_\alpha(r) \).

Yet further obfuscation occurs within the EDA which states that \( A_T(x) \approx A_T(0) \) whenever \( |x| \leq |r| \). This implies that \( \chi_\alpha \) in Eq. (11) is approximated as in Eq. (74). Thus, choosing the multipolar gauge, \( A_1 \), means choosing \( A_L = \nabla \chi_1 \) such that \( A_1(r) = -A_T(r) \) within the EDA, giving \( A_1(r) \approx 0 \) [cf. Eq. (86)]. The position \( r \) is of course where the potential \( A_1 \) is evaluated within the Hamiltonian [cf. Eq. (22)]. Thus, the dipole approximation of the kinetic energy part of the multipolar-gauge Hamiltonian is independent of the potential and the canonical momentum \( p \) becomes purely mechanical; \( p = m \dot{r} \). This again, may lead to the false impression that the multipolar Hamiltonian is not a minimal-coupling Hamiltonian.

Crucially, according to the gauge principle all Hamiltonians \( H_\alpha \) are equally valid, and any one of them can be taken as the starting point for a canonical description of QED. It is certainly not the case that only one particular gauge’s Hamiltonian, such as \( H_0 \), is compatible with the gauge-principle. Indeed, such a conclusion would contradict the gauge-principle. In particular, it is not the case that \( H_0(t) \) is a fundamentally preferable starting point when considering time-dependent interactions and that any other Hamiltonian must be obtained from it via a time-dependent gauge transformation. This fact appears to contradict recent articles [7, 10]. Time-dependent interactions are discussed in detail in Sec. IV.
J. Quantum subsystem relativity

The different ways of sharing out the constrained degrees of freedom has important implications when using the theory. To show this we first examine fundamental concepts relating to composite quantum systems and subsequently relate them to gauge-freedom.

In quantum theory all predictions are obtained from the inner-product, therefore the following associations

\[
\text{physical state } S \leftrightarrow \text{vector } |\psi\rangle \\
\text{physical observable } O \leftrightarrow \text{operator } O
\]

are equivalent to the associations

\[
\text{physical state } S \leftrightarrow \text{vector } |\psi'\rangle = U |\psi\rangle \\
\text{physical observable } O \leftrightarrow \text{operator } O' = UOU^\dagger
\]

where \(U\) is any unitary operator \([59]\). The definition of a composite quantum system uses the tensor-product \(\otimes\), which extends the inner-product in the way that is required in order that probabilities associated with independent subsystems are statistically independent. Specifically,

\[
\langle \psi_A | \otimes | \varphi_B \rangle \otimes | \varphi_B \rangle = \langle \psi_A | \varphi_A \rangle \langle \psi_B | \varphi_B \rangle.
\]

Quantum subsystems defined mathematically using \(\otimes\), are inherently relative. To see how, consider a composite system of two spins \(A\) and \(B\). We denote the states \(|\pm\rangle\) respectively, such that the states \(|\pm\rangle\) in Eq. (95), an entangled state? The answer is yes it is entangled with respect to the observables \(O_A\) and \(O_B\), and no it is not entangled with respect to the observables \(O_A\) and \(O_B\). Importantly, this is a physical statement regarding states and observables, which does not rely upon reference to vectors and operators. The state \(S_+\) is simultaneously entangled and not entangled because subsystems are relative. The term “entanglement” is referring to different physical observable properties within the two different answers to the question. Of course, both answers are correct and certainly not incompatible. We can further ask: is the entanglement in the state \(S_+\) physically relevant? The answer is yes if we are able to access observables \(O_A\) and \(O_B\), and the answer is no if we are only able to access the observables \(O_A\) and \(O_B\). This again, is a statement about physical states and observables without reference to vectors and operators. It also concerns what is actually measurable.

We initially assumed that \(O_A\) and \(O_B\) were represented by \(\sigma_A \otimes I_B\) and \(I_A \otimes \sigma_B\), which after transformation by \(U\), were used to represent \(O_A\) and \(O_B\). Thus, we have represented two distinct operational subsystems using the same mathematical subsystems. Operational subsystems are defined by their observables independent of how the latter are represented using operators, whereas mathematical subsystems are determined by the form that operational subsystems are represented in the fixed-gauge-fixing transformations \(U\).

K. Gauge-ambiguities and gauge-invariance

Quantum theory provides predictions for observables and the unitarity of gauge-fixing transformations \(U_{gg'}\) guarantees the gauge-invariance of these predictions. We define gauge-invariance as follows:

- A prediction is gauge-invariant if it is independent of the gauge in which it is calculated. If all predictions pertaining to an observable are gauge-invariant then the observable is gauge-invariant.

In general, an observable \(O\) is represented in the fixed-gauge \(\alpha\) by a generally \(\alpha\)-dependent function \(\alpha_{\alpha}(y)\) of the canonical operators \(y = \{r, A_T, p, \Pi\}\). A physical state \(\psi\) is represented by an \(\alpha\)-dependent vector \(|\psi_{\alpha}\rangle\). In the gauge \(\alpha'\), the same observable \(O\) is represented by the operator \(\alpha_{\alpha}(r_{\alpha\alpha'}y_{\alpha\alpha'}R_{\alpha\alpha'}^\dagger)\), which is the same state \(S\) is represented by the vector \(|\psi_{\alpha'}\rangle = R_{\alpha\alpha'}|\psi_{\alpha}\rangle\). Clearly the average \(\langle O \rangle_S\) can be calculated in any gauge

\[
\langle \psi_{\alpha} | o_{\alpha}(y) | \psi_{\alpha} \rangle = \langle O \rangle_S = \langle \psi_{\alpha'} | o_{\alpha'}(y) | \psi_{\alpha'} \rangle.
\]

This gauge-invariance holds as a consequence of the unitarity of gauge-fixing transformations and so it should be clear that it will hold independently of any restriction on the form of the gauge.
• In canonical non-relativistic QED, all physical observables and predictions are gauge-invariant.

An example of a gauge-invariant observable is the total energy $O = E$, which in the gauge $\alpha$ is represented by the Hamiltonian function $H_\alpha(y)$.

Although QED is fundamentally gauge-invariant, the task remains of deciding which observables are relevant to us. The transformation $U_{g\alpha'}$ does not have the form $U_{g\alpha'} = U_A \otimes U_B$ with respect to any tensor-product structure that can be imposed on the theory’s Hilbert space. Thus, different gauges do not produce equivalent mathematical subsystems. To understand the implications of this let us consider the observables $E_T$ and $P_T$ where hereafter we use $P_T \equiv P_{T1}$ to denote the multipolar transverse polarisation and correspondingly we use $P$ to denote the total multipolar polarisation. The transformation $R_{\alpha\alpha'}$ commutes with $P_T$, so this observable possesses the same operator representation in every gauge. The same is not true for $E_T$.

Let $\alpha$ denote a fixed real number that has nothing to do with the choice of gauge. Now consider the physical observable $O := -E_T - \alpha P_T$, which as a fixed linear combination of gauge-invariant observables is also gauge-invariant. Finally, let us suppose that we choose our gauge-parameter to have the same fixed value $\alpha$ as was used to define $O$. It happens then that the observable $O$ is represented by the operator $\Pi$. We emphasise that gauge-freedom is not a freedom to define $O$. It is a freedom to decide whether the parameter that fixes the redundancy $A_L$ within our description, equals the number $\alpha$ that defines $O$.

If the gauge parameter is instead chosen to have value $\alpha' \neq \alpha$, then $O$ is not represented by $\Pi$, which instead represents the gauge-invariant physical observable $O' := -E_T - \alpha' P_T$. Hence, in the gauge $\alpha'$ the physical observable $O$ is represented by the operator $\Pi' = R_{\alpha\alpha'} \Pi R^{\dagger}_{\alpha\alpha'} - (\alpha - \alpha')P_T$. A physical state $S$ is represented by the vectors $|\psi\rangle$ and $|\psi'\rangle = R_{\alpha\alpha'} |\psi\rangle$ in the gauges $\alpha$ and $\alpha'$ respectively. Thus, the averages of $O$ and $O'$ in the state $S$ are

$$\langle O \rangle_S = \langle \psi | \Pi | \psi \rangle, \quad (97)$$
$$\langle O' \rangle_S = \langle \psi' | \Pi | \psi' \rangle. \quad (98)$$

The same operator $\Pi$ represents different observables $O$ and $O'$ in the two averages, whereas different vectors represent the same physical state $S$. Of crucial importance is to recognise that both of the above predictions are examples of predictions that satisfy gauge-invariance as defined by Eq. (96). However, they are clearly different physical predictions even though both are averages of an operator $\Pi$, which defines the “light” quantum subsystem.

For fixed $\alpha$ the combination $\Pi = -E_T - \alpha P_T$ is a gauge-invariant observable, but by definition of $\Pi$, the gauge parameter $\alpha$ is the gauge parameter. Thus, while it is true that in each gauge $\Pi$ represents a physical observable and while it is also true that every observable possesses unique physical predictions that can be calculated in any gauge, it is not true that the operator $\Pi$ represents the same physical observable in any two different gauges, and naturally:

• Different observables have different predictions.

For example, the physical predictions $\langle O \rangle_S$ and $\langle O' \rangle_S$ in Eqs. (97) and (98) respectively are both found using $\Pi$ and both are gauge-invariant, but they are clearly different. The task remains of determining which of these gauge-invariant predictions is relevant in which situations. As will be discussed throughout the present article, this task is intimately related to the interpretation of virtual particles and processes, and to locality.

On a practical level, simply verifying the fundamental gauge-invariance of predictions does not imply that gauge-freedom can be ignored. For example, Ref. [10] (Sec. V) notes that “of course detectable subsystem excitations and correlations have to be gauge-invariant, since the results of experiments cannot depend on the gauge. On this basis we can define gauge invariant excitations and qubit-field entanglement”. We note however, that providing gauge-invariant definitions is straightforward and this has never been a problem. Indeed, given the unitarity of gauge-fixing transformations, gauge-invariance is automatic. “Ambiguities” occur not because gauge-invariance breaks down, but because there are many different gauge-invariant definitions of “excitations and qubit-field entanglement”. The latter can be defined relative to any gauge (see Sec. II L). Gauge-invariance is necessary, but it is not a sufficient “basis” for providing physically relevant theoretical definitions. Any conceptual ambiguities that result from the availability of many different physical definitions can be called “gauge-ambiguities”, but they are not due to a breakdown of gauge-invariance, which is a fundamental requirement.

L. Definition of subsystem gauge relativity

We adopt the viewpoint that the relevant definition of any system is determined by experimental capability. Operationally, a “system” comprises a set of observable properties that can be measured. On the other hand, theoretically there exists a continuous infinity of different gauge-invariant transverse fields, all of which are represented by the operator $\Pi$. Any of these fields can be used to define a spin-1 massless boson called a photon. Mathematically, “photons” are defined directly in terms of $\Pi$ via

$$a_\lambda(k) := \frac{1}{\sqrt{2\omega}} e_\lambda(k) \cdot [\omega \hat{A}_T(k) + i\bar{\Pi}(k)] \quad (99)$$
where \( \omega := |k| \) and \( e_\lambda(k) \) is a unit polarisation vector orthogonal to \( k \) (Fourier transforms are denoted with a tilde). From \( \Pi = -E_T - \alpha P_T \), it is clear that for each different fixed value of \( \alpha \) the photon number operator \( n = \sum_{k\lambda} a_\lambda^\dagger(k) a_\lambda(k) \) represents a different gauge-invariant observable:

- Photons defined using the gauge-invariant observable \( O = -E_T - \alpha P_T \), which in the gauge \( \alpha \) is represented by the operator \( \Pi \), are said to be defined relative to the gauge \( \alpha \).

The eigenstates of the corresponding number operator \( n \) are a basis for the “light” Hilbert space. Thus, the mathematical “light” subsystem is defined relative to a choice of gauge. We can express this relativity symbolically by writing the subsystem label “light” as a function of the observable that defines it, for instance, in the gauge \( \alpha \): \( \text{light}(E_T + \alpha P_T) =: \text{light}_\alpha \). As an example, suppose that in a given experiment the observable \( E_T \) is measurable, then evidently \( \text{light}_\alpha \) is at least one relevant mathematical subsystem for describing this experiment.

To summarise, according to the postulates of quantum theory, QED subsystems are mathematically defined using the tensor-product, and therefore by the canonical operators, which represent different physical observables in each different gauge [4]. It follows that

- QED subsystems are defined relative to a choice of gauge [4].

Although subsystems are gauge-relative, physical predictions will always be gauge-invariant if they are calculated properly [cf. Eq. (96)] and approximations that ruin gauge-invariance are avoided. For example, to obtain gauge-invariant predictions when dealing with time-dependent interactions one must of course take into account the time-dependence of gauge transformations, as noted in Refs. [5, 10]. However, doing so does not mean that gauge-ambiguities do not arise.

Ambiguities arise because it is not always clear that any one definition of photon, for example the definition using \( E_T \), is the most physically relevant definition. These conceptual difficulties can be avoided in traditional weak-coupling and Markovian regimes, as will be clearly demonstrated in Sec. IV, but they cannot generally be ignored in, for example, the ultrastrong-coupling regime.

M. Implications

The subsystem gauge-relativity of canonical QED is a form of linear-space relativity analogous to that encountered in theories of space and time. The definition \( \text{light}_\alpha \) is not directly relevant for predicting the outcome of a measurement of the photons that define \( \text{light}_\alpha \), except in a regime where the mixing of “light” and “matter” due to the gauge-transformation \( R_{\alpha \alpha'} \) can be ignored. This latter situation is often encountered in the regime of weakly-coupled, nearly-resonant, and Markovian systems [5], as will be demonstrated directly in Sec. IV. Within sufficiently strong-coupling regimes, the task of determining which gauge-invariant mathematical definition of “photon” is most relevant for predicting the outcome of an actual photon measurement, is not necessarily straightforward.

Ref. [10], for example, assumes that a photodetector registers photons defined by the gauge-invariant transverse electric field \( E_T \). Given this assumption about which physical observable is relevant, one can of course calculate the rate of photodetection as a unique physical prediction in any gauge for both time-dependent and time-independent interactions. In Glauber’s original theory however, the total electric field \( E = E_T + E_L \) was used [26, 60]. The total field is only transverse when there are no charges present. As we have already noted, recognising the distinction between \( E_T \) and \( E \) is essential and lies at the heart of gauge-ambiguities. It has been argued in the past that the transverse displacement field \( D_T = E_T + P_T \) provides the relevant definition, because its source-component equals the source-component of \( E \) away from the source, and it is therefore local, unlike \( E_T \) [24–31]. It has been known for six decades that photons defined relative to the multipolar-gauge, i.e., in terms of \( D_T \), provide a natural lineshape prediction that are in sufficient agreement with early experiments to rule out the prediction for the same experiments when photons are defined using \( E_T \) [33–36]. For these specific experiments the multipolar-gauge subsystems are evidently more operationally relevant than the Coulomb-gauge subsystems.

However, in QED one typically views physical particles as being dressed by virtual photons and this is more consistent with definitions provided by \( \alpha \neq 1 \) whereby the quantum dipole is not purely “bare” and localised, but is instead a delocalised dressed object. Conversely, only the multipolar-gauge provides a definition of the dipole to which a test charge placed away from the dipole centre at \( 0 \) does not respond instantaneously [24–31]. In gauges \( \alpha \neq 1 \) the extent of the apparently instantaneous, but typically small response of a test charge distribution to the field of the \( \alpha \)-gauge dipole could simply be interpreted as a measure of the dressed dipole’s delocalisation due to its own virtual cloud of photons [61]. These points are discussed in the context of photodetection theory in Sec. V.

For given values of the remaining model parameters, it is always possible to choose an intermediate value of \( \alpha \) denoted \( \alpha_{JC} \), which lies between 0 and 1, and for which ground state virtual photons are highly suppressed [4]. This can be interpreted as identifying a representation in which such photons have been absorbed into the definitions of the quantum subsystems. The physical meanings of the different mathematical definitions of “light” and “matter” are evidently closely related to virtual photons and processes.

Finally we note that a prosaic implication of subsystem gauge-relativity is that approximations performed on the
subsystems can ruin the gauge-invariance of the theory. A well-known example is the truncation of the material system to a finite number of levels [4, 7–9]. Because “matter” is defined differently in different gauges, the truncation generally constitutes a significantly different physical procedure in different gauges. This is discussed in detail in Sec. III.

N. Gauge-freedom and duality symmetry

Recently a novel derivation of the multipolar Hamiltonian has been provided using a dual potential as coordinate with the aim of addressing certain gauge-ambiguities [62]. We briefly review this approach. The dual-potential $C_T$ is such that

$$C_T(x) = -(\nabla \times)^{-1} \Pi(x) = -\int d^3x' \frac{\nabla' \times \Pi(x')}{{4\pi}|x-x'|}.$$  \hfill (100)

In the same way that $A_T$ is conjugate to $\Pi$ the potential $C_T$ can be viewed as a coordinate conjugate to the magnetic field $B$, because as is easily verified

$$[C_{T,i}(x), B_j(x')] = i\delta_{ij}(x-x').$$  \hfill (101)

Due to the non-existence of magnetic charge, as specified by $\nabla \cdot B = 0$, the magnetic quantities $A_T$ and $B = \nabla \times A_T$ are physically unique. In contrast, due to Gauss’ law $\nabla \cdot E = \rho$, which generates gauge-symmetry transformations [Eq. (33)], the electric quantities $C_T$ and $\Pi = -\nabla \times C_T$ represent different observables in different gauges. The field canonical subsystem is defined using $(A_T, \Pi)$ or equivalently using $(C_T, B)$. Since the curl operator, $\nabla \times$, is invertible on the space of transverse fields [cf. Eq. (100)], any function of $(A_T, \Pi)$ can instead be written as a function of $(C_T, B)$ and vice versa. The $\alpha$-gauge Hamiltonian given in Eq. (22) can be written in terms of $C_T$ and $B$ using $\Pi = -\nabla \times C_T$ and Eq. (84).

Choosing the multipolar-gauge, $\alpha = 1$, then gives the result of Ref. [62]. Ref. [62] refers to gauge-freedom as a freedom to choose $C_L$. This freedom has no non-trivial consequences in the absence of magnetic charge, and it is independent of the gauge-freedom in $A_L$. The latter freedom is highly non-trivial and it is necessarily present as a fundamental feature of QED. An expression of the theory in terms of $(C_T, B)$ is always possible, but this cannot circumvent gauge-freedom in $A_L$. However, when written in terms of dual coordinates the dependence of the theory on $A_L$ is no longer explicit. The freedom within the theory is understood in terms of the “polarisation” $P$ and the accompanying “magnetisation” $M$ (defined in Appendix VI), which are auxiliary potentials for the charge and current densities $\rho$ and $J$.

Ref. [62] argues that the potentials $P$ and $M$ may offer a more intuitive way to understand the relativity within the light-matter subsystem decomposition. It must however be noted that $P_T$ is completely arbitrary and once fixed determines $M$, in the same way that $A_1$ is completely arbitrary and once fixed determines $A_0$. As noted in Sec. II C, a gauge transformation of $P_T$ as defined in Eq. (59) is necessarily accompanied by a gauge transformation in $A_L$ [Eq. (58)].

Ref. [62] concludes that approximations within the multipolar-gauge, $\alpha = 1$, will typically most accurately represent the physics of small, bound dipoles interacting with a single mode. A wide range of system types is considered along with the effects of both material truncation and the EDA. However, it has been noted elsewhere that while the multipolar-gauge may often be optimal (or very close to optimal) for performing material level truncations, this is not always the case when considering low energy properties involving more than one radiation mode or less anharmonic material dipoles [4, 8].

Most importantly, it is essential to recognise that gauge ambiguities are much broader than the gauge non-invariance resulting from approximations, which are always avoidable in principle. As we have shown the canonical dipole defined by $(r, p)$ possesses a continuously varying level of localisation directly controlled by the gauge. The strict multipolar dipole is unphysical due to its singular nature. The interplay between localisation and dressing is directly relevant in determining measurable properties. In particular, the distinction between real and virtual photons is important and is intimately related to the choice of gauge. These points are discussed in detail in the context of time-dependent interactions in Sec. IV and photodetection theory in Sec. V. It is shown that the multipolar-gauge may yield especially unphysical results in photodetection theory.

O. Modal restrictions and transversality

Restrictions on the number of photonic modes are extremely common in light-matter physics. However, retaining all modes is necessary to properly maintain certain spacetime properties such as localisation and causal wave propagation [63]. In particular, the green’s function for the wave operator receives contributions from all $k$-space-modes. Thus, a modal restriction should only be understood as a statement about which particular frequencies are dominant within a given light-matter interaction Hamiltonian. We briefly discuss the implementation of such restrictions here.

1. Significance of transversality

We begin by noting that the transversality of canonical fields is an important aspect of Hamiltonian QED closely related to gauge-freedom. Only transverse fields can be used to define unconstrained physical photons as in Eq. (99). This feature is fundamental and it persists in a generalised sense in the presence of background media, as are relevant in numerous artificial photonic systems.
that realise strong-coupling [64–69]. All massless representations of the Lorentz group result in fields with only two independent degrees of freedom. In particular, the massless spin-1 Maxwell field supports the two independent polarisations of a photon. Scalar and longitudinal photons can also be defined, as in the Lorentz-gauge (also called Lorenz-gauge), but such photons are not constrained, they must satisfy a non-dynamical constraint (Lorentz subsidiary condition), whose derivative in time is Gauss’ law [24].

Gauss’ law generates gauge-symmetry transformations and its derivative in time is the continuity equation for electric charge, which is the conserved quantity associated with gauge-symmetry. Gauss’ law specifies $\mathbf{E}_L$ as a function of $\rho$, which tells us that longitudinal photons are not independent. Specifically, an analog of Eq. (99) may be written

$$a_L(k) := -\frac{i}{\sqrt{2\omega_k}} \mathbf{k} \cdot \mathbf{E}(k) = -\frac{i}{\sqrt{2\omega_k}} \mathbf{E}.$$  \hspace{1cm} (102)

Although $\mathbf{E}_T$ is the part of the electric field not constrained by Gauss’ law, it is by fundamental assumption that the total electric field $\mathbf{E}$ is local. It follows that the fields $\mathbf{E}_L$ and notably $\mathbf{E}_T = \mathbf{E} - \mathbf{E}_L$, are both non-local [cf. Eq. (7)] and away from a localised source they respond instantaneously to changes in the source [24, 53]. The multipolar-gauge momentum $\Pi = -\mathbf{D}_T$ offers the best possible representation of the non-transverse local field $\mathbf{E}$ by an unconstrained transverse field that can then be used to define unconstrained photons [24]. Specifically, $\mathbf{P}_L = -\mathbf{E}_L$ implies that $\mathbf{D} := \mathbf{E} + \mathbf{P} = (\mathbf{E}_T + \mathbf{E}_L) + (\mathbf{P}_T - \mathbf{E}_L) \equiv \mathbf{D}_T$ and since $\mathbf{P}$ vanishes outside of a charge distribution we have $\mathbf{D} \equiv \mathbf{D}_T = \mathbf{E}$ at all such points. It is certainly not the case however that $\mathbf{E} = \mathbf{E}_T$ nor that $\mathbf{P} = \mathbf{P}_T$.

In the case of a dipole at $0$ we have $\mathbf{P} = q \mathbf{r} \delta(x)$ whereas $\mathbf{P}_T(x) = q \mathbf{r} \cdot \delta^T(x)$. The transverse dyadic $\delta^T(x)$ is not purely singular, rather it decays as $1/x^3$ away from $0$. From elementary electrostatics we know that $\mathbf{E}_L$ decays as $1/x^3$ away from a dipole at $0$ and for a dipole we do indeed have $\mathbf{P}_T = \mathbf{E}_L$ for $x \neq 0$ (i.e., $\mathbf{P}(x) = q \mathbf{r} \delta(x) = 0$ for $x \neq 0$). For any $\alpha$ the field $\Pi$ can be expanded in terms of photons using Eq. (99). Crucially however, for different $\alpha$ these fields are related by the non-local field $\mathbf{P}_T$.

For a transverse field, the mode functions $f_\lambda(k, x) = e^{ik \cdot x}/\sqrt{2\pi}$ of a canonical mode-expansion are not complete with respect to the usual inner-product in $L^2(\mathbb{R}^3)$, because $\{e_\lambda(k)\}$ is an orthonormal basis in the two-dimensional plane orthogonal to $k$. Instead they furnish a representation of the transverse delta function;

$$\int d^3k \sum_{\lambda=1,2} f_\lambda(k, x)^* f_\lambda(k, x') = \delta^T(x - x').$$  \hspace{1cm} (103)

To obtain a representation of $\delta(x - x')$ one must add $k$ to the 3-dimensional basis $\{k, e_\lambda(k)\}$. If the longitudinal eigenfrequency is set to vanish $\omega_L = 0$ then one can expand $\Pi$ using the complete set of mode functions as

$$\Pi(x) = i \int d^3k \sum_{\lambda=1,2,L} \sqrt{\frac{\omega_\lambda}{2}} \times [f_\lambda(k, x)^* a_\lambda^\dagger(k) + f_\lambda(k, x) a_\lambda(k)]$$  \hspace{1cm} (104)

where $\omega_{1,2} \equiv \omega$. However, the operators $a_\lambda(k)$ have completely arbitrary definition and cannot contribute to physical predictions.

2. Modal restriction

Ultrastrong-coupling between light and matter arises in artificial systems in which the set of photonic modes is altered and often restricted. Theoretically, care must be taken when carrying out such restrictions. To demonstrate this we choose the multipolar-gauge, such that $\Pi = -\mathbf{D}_T$, implying that the Coulomb-gauge momentum $-\mathbf{E}_T$ is represented by the operator $\Pi' = -\mathbf{E}_T = R_{10} \Pi R_{10}^\dagger = \Pi + \mathbf{P}_T$. Coulomb and multipolar-gauge transverse photonic operators $a^\dagger_\lambda(k)$ and $a_\lambda(k)$ are defined as in Eq. (99) using $\Pi' = -\mathbf{E}_T$ and $\Pi = -\mathbf{D}_T$ respectively. They are therefore related by

$$a^\dagger_\lambda(k) = R_{10} a_\lambda(k) R_{10}^\dagger = a_\lambda(k) + \frac{q \mathbf{r} \cdot f_\lambda(k, 0)}{\sqrt{2\omega_\lambda}}.$$  \hspace{1cm} (105)

For the unphysical longitudinal mode operators any relation can be specified. We note however, that the right-hand-side of Eq. (105) would be undefined for $\lambda = L$, because $\omega_L \equiv 0$. The total electric field is given by $\mathbf{E} = -\mathbf{D}_T - \mathbf{P} = -\Pi - \mathbf{P} = -\Pi' - \mathbf{P}_L$ and $\mathbf{P}(x) = q \mathbf{r} \delta(x)$ is fully localised. $\mathbf{E}$ is completely independent of the $a_\lambda(k)$, as any physical field must be.

By discretising the modes in a volume $v$ the mode functions become discrete $f_\lambda(k, x) \rightarrow f_\lambda(k)$ such that factors of $(2\pi)^3$ are replaced by $v$. For $\lambda = 1, 2$ the fields associated with the wavevector $k$ are

$$\Pi_k(x) = -\mathbf{D}_{Tk}(x) = i \sum_{\lambda=1,2} \sqrt{\frac{\omega}{2}} (f_{k\lambda}(x)^* a_{k\lambda}^\dagger - \text{H.c.})$$

$$= \Pi_k'(x) - \mathbf{P}_{Tk}(x),$$  \hspace{1cm} (106)

$$\Pi_k'(x) = -\mathbf{E}_{Tk}(x) = i \sum_{\lambda=1,2} \sqrt{\frac{\omega}{2}} (f_{k\lambda}(x)^* a_{k\lambda}^\dagger - \text{H.c.})$$

$$\mathbf{P}_{Tk}(x) = q \mathbf{e}_{k\lambda} \frac{\mathbf{e}_{k\lambda} \cdot \mathbf{r}}{v} \cos k \cdot x.$$  \hspace{1cm} (107)

Meanwhile for $\lambda = L$ we have

$$\mathbf{E}_{Lk}(x) = -q \mathbf{k} \frac{\mathbf{k} \cdot \mathbf{r}}{v} \cos k \cdot x = -\mathbf{P}_{Lk}(x).$$  \hspace{1cm} (109)

The corresponding restricted total polarisation and total electric fields are

$$\mathbf{P}_k(x) = \mathbf{P}_{Tk}(x) + \mathbf{P}_{Lk}(x) = \frac{q \mathbf{r}}{v} \cos(k \cdot x),$$

$$\mathbf{E}_k(x) = -\Pi_k'(x) - \mathbf{P}_{Tk}(x) = -\Pi_k(x) - \mathbf{P}_k(x).$$  \hspace{1cm} (111)
The approximation as given above in the form \( V \) must be understood as an assumption about which modes within the Hamiltonian of a light-matter system remain unitary and are given by [4, 5]

\[
A_\alpha = (1 - \alpha)A = \frac{1 - \alpha}{\sqrt{2\omega v}}(a^\dagger + a)
\]

\[
P_{\alpha\alpha'} = \frac{\alpha q_x}{v}.
\]

Here \( x = \epsilon \cdot r \) and \( A = \epsilon \cdot A_T(0) \) where \( \epsilon \) is the unit polarisation vector of the single transverse mode retained. Within these approximations the Hamiltonian reduces to the simple form that has now been used in a number of works [4–8]. The gauge-fixing transformations \( R_{\alpha\alpha'} \) in Eq. (77) remain unitary and are given by [4, 5]

\[
R_{\alpha\alpha'} = \exp(i[\alpha - \alpha']q_x A).
\]

The approximation of restricting to a finite-number of modes within the Hamiltonian of a light-matter system must be understood as an assumption about which modes are dominant within the dipole-field interaction. Such an approximation as given above in the form \( V(0) = \sum_k V_k(0) \approx V_k(0) \) could be valid at the position of the dipole, \( 0 \), which is where any field is evaluated within the interaction Hamiltonian. However, this is also where the field cannot be measured by an external detector. For any \( x \) the field \( E_k \) equals neither \( -E_{Tk} \) nor \( -D_{Tk} \). Due to Gauss’ law the electric-field, whether restricted or not, cannot be expressed solely in terms of physical (transverse) photons. In particular, since \( \Pi_k \) is orthogonal to \( k \), one cannot obtain \( E_k \) by means of a unitary operator acting on \( \Pi_k \).

Obviously the fully localised physical polarisation \( P(x) = \sum_k P_k(x) \) cannot be elicited in a restricted space of wave-vectors. A modal restriction at an arbitrary point \( x \neq 0 \) will therefore violate the property \( P_T = -P_L \) of the full theory. Naively restricting Eqs. (110) and (111) to only one transverse mode \( k \lambda \) means \( P_{Tk}(x) \equiv 0 \) and we obtain \( E_{k\lambda}(x) = -\Pi_{k\lambda}(x) = -\Pi_{k\lambda}(x) - P_{Tk\lambda}(x) \). This yields a theory without \( E_L \), that can therefore only be valid in the far-field. Of course, in the far-field where \( E_L = P_T \) vanishes, we have \(-\Pi' = E_T \approx E = -\Pi \) whether or not the modes are restricted. If we instead use the fact that \( \Pi(x) = -E(x) \) for \( x \neq 0 \) and then restrict our attention to one transverse mode, we obtain the different result \( E_{k\lambda}(x) \equiv -\Pi_{k\lambda}(x) = -\Pi_{k\lambda}(x) + P_{Tk\lambda}(x) \). This single-mode limit respects the equalities \( E = -\Pi = -\Pi' + P_T \) holding for \( x \neq 0 \) in the unrestricted theory. We note that within the light-matter interaction Hamiltonian, physical fields are evaluated at \( x = 0 \) so the above considerations do not apply.

Evidently, different implementations of a modal restriction can result in altogether different identifications of the same physical field, such that care must be taken in restricting the modes. In the above case of the electric field \( E \) we have fundamentally that at all points \( x \) outside of a charge distribution, which is where the field can be measured by an external detector, the physical polarisation vanishes, implying that at such points \( \Pi(x) = -E(x) \) in and only in the multipolar-gauge. We should not expect a modal restriction in which this is no longer the case to offer a generally robust approximation of the unrestricted theory for describing measurements in the vicinity of \( x \). In particular, since the field \( (t, x) \) is given within the single-mode limit that respects the fundamental equalities of the multi-mode theory by

\[
\langle E_{k\lambda}^-(t, x) \cdot E_{k\lambda}^+(t, x) \rangle = \frac{\omega}{2v} \langle a_{k\lambda}^\dagger(t) a_{k\lambda}(t) \rangle
\]

where \( a_{k\lambda} \) is the multipolar-gauge photonic operator. Irrespective of modal restrictions, the Glauber intensity is not proportional to the photon number operator defined relative to the Coulomb-gauge except in the far-field where we have \( E \approx E_T \). Photodetection is discussed in detail in Sec. IV. We note that the considerations of this section also apply in the case of dispersive and absorbing media important for polaritonic systems that realise ultrasstrong light-matter interactions. In this case canonical fields remain transverse [70].

P. Simple extension to superconducting circuits

The arbitrary-gauge formalism is readily adapted to describe circuit QED systems. We briefly review this here, including how gauge-freedom manifests. Conventional descriptions of superconducting circuits employ the lumped-element model, which results from Kirchhoff’s assumptions applied to Maxwell theory. Consider a node defined as the meeting point of \( N \) conducting wire branches outside of which there is no current. Bounding the node is a closed surface \( S \) containing a region \( v \) with outward normal \( \hat{n} \). The continuity equation \( \partial_r j^\nu = 0 \) and divergence theorem yield

\[
\sum_{\mu=1}^N I_\mu(t) = \sum_{\mu=1}^N \int_{S_\mu} dS \hat{n} \cdot J(t, x) = -\frac{dQ(t)}{dt},
\]

(116)

\[
Q(t) = \int_v d^3x \rho(t, x),
\]

(117)

where \( S_\mu \) is the subsurface of \( S \) intersecting the \( \mu \)th wire, \( I_\mu \) is the current entering \( v \) through the \( \mu \)th wire, and \( Q(t) \) is the total charge within the region \( v \) containing the node. Eq. (116) assumes that \( J(t, x) = 0 \) for all \( x \in S \setminus \bigcup_\mu S_\mu \) (there is no current outside the conducting wires). Kirchhoff assumed further a local steady-state current condition within \( v \), namely, \( dQ(t)/dt = 0 \), yielding the current law

\[
\sum_{\mu=1}^N I_\mu(t) = 0.
\]

(118)
FIG. 1: Circuit diagram for a parallel LC-oscillator coupled to a series LC-oscillator. There are three nodes within the circuit. The subfigures each provide a different labelling of the nodes corresponding to different specifications of the ground flux. As a result, they depict two different divisions of the circuit into subsystems. Specifically, these are the two extreme cases of (a) fully inductive coupling whereby the ground flux is specified as the flux associated with the node that is labelled \( g \), and (b) fully capacitive coupling whereby the ground flux is specified as the flux associated with the node that is labelled by \( g' \).

Arbitrary lumped-element circuits can be considered as collections of nodes joined by (superconducting) branches, with Kirchoff’s law, Eq. (118), satisfied at each node. As a non-trivial example we consider the coupled LC-oscillator circuit depicted in Fig. 1 (a). As basic dynamical variables we take the node fluxes denoted \( \phi_k \). The current into node \( k \) through a branch \( j \rightarrow k \) with an inductor connecting node \( k \) to node \( j \) is \( I_{j\rightarrow k} = (\phi_k - \phi_j)/L \) where \( L \) is the inductance of the inductor. The current into node \( k \) through a branch \( j \rightarrow k \) with a capacitor connecting node \( k \) to node \( j \) is \( I_{j\rightarrow k} = C(\phi_k - \phi_j) \) where \( C \) is the capacitance of the capacitor. Since only flux differences are of importance we can specify the flux zero-point arbitrarily. This is the so-called ground flux such that \( \phi_g = 0 \). As particular special cases, we can choose this flux zero-point to be the flux of one of the circuit nodes depicted in Fig. 1 wherein subfigures (a) and (b) give two different specifications of which node possesses the ground flux.

In the circuit of Fig. 1 (a) there are two non-ground nodes labelled \( m \) and \( c \). Kirchoff’s law, Eq. (118), yields the equations of motion

\[
0 = I_{g\rightarrow m} + I_{c\rightarrow m} = C_m \dddot{\phi}_m + \frac{\phi_m}{L_m} + \frac{\phi_m - \phi_c}{L_c},
\]

\[
0 = I_{g\rightarrow c} + I_{m\rightarrow c} = C_c \dddot{\phi}_c + \frac{\phi_c - \phi_m}{L_c}.
\]

These equations of motion are obtained from the Lagrangian

\[
L = \frac{1}{2} \left[ C_m \dddot{\phi}_m^2 - \frac{\phi_m^2}{L_m} + C_c \dddot{\phi}_c^2 + \frac{(\phi_c - \phi_m)^2}{L_c} \right]
\]

or corresponding Hamiltonian

\[
H = \frac{1}{2} \left[ C_m \dot{q}_m^2 + \frac{\dot{q}_m^2}{L_m} + C_c \dot{q}_c^2 + \frac{(\phi_c - \phi_m)^2}{L_c} \right]
\]

where \( q_x = \partial L/\partial \dot{\phi}_x \) are the node charges conjugate to the \( \phi_x \) with \( x = m, c \). A node flux and its conjugate charge satisfy a canonical Lie bracket relation, which generates the dynamics in conjunction with the Hamiltonian. In particular, in the quantum theory, \( [\phi_x, q_{x'}] = i\hbar \delta_{xx'} \).

Let us now consider a relabelling of the nodes as depicted in Fig. 1 (b). The ground node has flux \( \phi_{g'} = 0 \) and the non-ground nodes \( m' \) and \( c' \) are now connected by the capacitance \( C_c \) rather than by the inductance \( L_c \). Since the physical currents through the branches must stay the same we obtain the coordinate relations

\[
\phi_{m'} = -\phi_m,
\]

\[
\phi_{c'} = \phi_c - \phi_m.
\]

Either \( \phi_m \) or \( \phi_{m'} \) can be used as a coordinate with \( \phi_{c'} \). We choose \( \phi_m \). The sum of Eqs. (119) and (120) can be expressed as

\[
0 = C_m \dddot{\phi}_m + C_c (\dddot{\phi}_m + \dddot{\phi}_c) + \frac{\phi_m}{L_m},
\]

and this equation together with Eq. (120) is obtained from the Lagrangian (121) or Hamiltonian (122) with \( \phi_m \) and \( \phi_{c'} \) taken as dynamical coordinates. At the Hamiltonian level the primed and unprimed canonical operators are related by a gauge-fixing transformation as

\[
q_{m'} = R_{10} q_m R_{10}^†,
\]

\[
\phi_{c'} = R_{10} \phi_c R_{10}^†
\]

where \( R_{10} := e^{-i\phi_m \phi_m} \).

This is analogous to the PZW transformation between the charge (Coulomb)-gauge and the flux (multipolar)-gauge.

Note that within the above derivation we have adopted a passive view of rotations within the operator algebra, by which we mean that the same Hamiltonian has been expressed in terms of alternative canonical operators that belong to different gauges. Equivalently, we may adopt an active perspective as in previous sections, whereby the Hamiltonian \( H \) is actively rotated using gauge-fixing transformations yielding new Hamiltonians which are all expressed in terms of the same canonical operators. The extension to arbitrary gauges is straightforward via the the gauge-fixing transformation

\[
R_{\alpha \alpha'} := e^{-i(\alpha - \alpha') \phi_c \phi_m}.
\]

We note that gauges specified by \( \alpha \neq 0 \), I do not correspond to a definite specification of one of the nodes within Fig. 1 as possessing the ground flux \( \phi_g = 0 \). Instead the ground flux is specified as some combination of the fluxes associated with the three nodes.

The basic non-linear element in superconducting circuits is the Josephson Junction. The formalism above
is easily extended to arbitrary circuits constructed from capacitors, inductors and Josephson junctions. For example, by adding a Josephson junction connecting the ground node $g$ to the node $m$ in Fig. 1, one obtains the light-matter Hamiltonian

$$H' = H - E_J \cos[2q\phi_m]$$  \hfill (130)

where the additional term $-E_J \cos[2q\phi_m]$ is the Josephson potential with energy $E_J$. The Hamiltonian $H'$ possesses the same structure as the cavity QED Hamiltonian considered in Sec. II A in which the material potential is arbitrary.

We have seen that the choice of gauge is determined by the choice of ground flux, and that arbitrary choices of gauge selected by a parameter $\alpha$ may be considered. Gauge-fixing transformations are directly analogous to those encountered in conventional QED, and as such, they are non-local with respect to Hilbert space tensor-product structure. A circuit may be dividing into physically distinct canonical sub-circuits arbitrarily and this division is directly controlled by the choice of gauge.

III. MATERIAL TRUNCATION AND GAUGE NON-INVARiance

Material energy level truncation is a commonly adopted procedure, that nevertheless breaks the gauge-invariance of QED by fundamentally modifying the algebra of material operators. This has been discussed in the context of strong and ultrastrong-coupling in Refs. [4–13]. Here we review the implications of the result of gauge invariance [4–6]. The dipole is assumed to be located at the origin $\mathbf{r}$ and for simplicity the canonical operators are assumed to point in the direction $\mathbf{e}$ of polarisation of the the single mode. They are specified entirely by scalar operator components in this direction. We define $x = \mathbf{e} \cdot \mathbf{r}$ and $A = \mathbf{e} \cdot \mathbf{A}_T$ and denote by $p$ and $\Pi$ the corresponding dipole and cavity canonical momenta, such that $[x,p] = i\hbar$ and $[A,\Pi] = i\hbar/v$ with $v$ the cavity volume. Details of the EDA and single-mode restriction are given in Secs. II F and II O 2 respectively.

The $\alpha$-gauge continues to be specified by its vector potential $A_\alpha = \mathbf{e} \cdot \mathbf{A}_\alpha$ and material polarisation $\mathbf{P}_{Ta} = \mathbf{e} \mathbf{P}_{Ta}$ which are given by Eqs. (112) and (113) respectively. The unitary gauge-fixing transformation $R_{\alpha\alpha'}$ between gauges $\alpha$ and $\alpha'$ is given by Eq. (114). The definition of gauge-freedom given by Eqs. (27) and (28) now reads

$$R_{\alpha\alpha'} p R_{\alpha\alpha'}^\dagger = p - (\alpha - \alpha') \mathbf{q}_A,$$  \hfill (131)

$$R_{\alpha\alpha'} \Pi R_{\alpha\alpha'}^\dagger = \Pi - (\alpha - \alpha') \mathbf{q}_F.$$  \hfill (132)

Since gauge-fixing transformations remain unitary the gauge-invariance of the theory is preserved. Were Eqs. (131) and (132) not satisfied, then $R_{\alpha\alpha'}$ would not effect the replacement $(A_p, P_{Ta}) \rightarrow (A_p^\prime, P_{Ta}^\prime)$, meaning it would not be a gauge-transformation from $\alpha$ to $\alpha'$. Note that since $U_f(O)U^\dagger = f(UO)U^\dagger$ for any unitary transformation $U$, suitably well-defined function $f$, and operator $O$, Eqs. (131) and (132) are necessary and sufficient to define how arbitrary functions of $p$ and $\Pi$ transform under a gauge-transformation.

The Hamiltonian is as ever the total energy, which is the sum of material mechanical and transverse electromagnetic energies [4, 5]:

$$H_\alpha = H_m(A_\alpha) + H_{ph,\alpha}$$  \hfill (133)

$$H_m(A_\alpha) := \frac{1}{2} m \dot{x}^2 + V(x) = \frac{1}{2m} (p - q A_\alpha)^2 + V(x),$$  \hfill (134)

$$H_{ph,\alpha} := \frac{v}{2} (E_{T}^2 + \omega A^2) = \frac{v}{2} [(\Pi + P_{Ta})^2 + \omega^2 A_T^2],$$  \hfill (135)

where $\dot{x} = -i[x, H_\alpha]$ and $E_T = -\dot{A}_T = i[A_T, H_\alpha]$. Hamiltonians of different gauges continue to be unitarily related as in Eq. (25). Certain non-fundamental properties of the Hamiltonian in Eq. (133) hold due to the simplifications that have been made. In particular, within the EDA the gauge-function $\chi_\alpha$ in Eq. (11) becomes that in Eq. (74), which gives $\nabla \chi_1(\mathbf{r}) = -\mathbf{A}_T(0)$, and so as noted in Sec. III one obtains $p - \mathbf{q}_A(\mathbf{r}) \approx \mathbf{p}$. Thus, letting $\alpha = 1$ on the left-hand-side of Eq. (27) we obtain $R_{10} p R_{10}^\dagger = p - \mathbf{q}_A$, where $\mathbf{A}_\alpha := (1 - \alpha) \mathbf{A}_T(0)$ is the EDA of $A_\alpha(\mathbf{r})$. In other words, within (and only within) the EDA the $\alpha$-gauge mechanical momentum may be obtained from the canonical momentum $\mathbf{p}$ using $R_{10}$.

Within the full 3-dimensional setting and without the EDA it is impossible to implement the minimal-coupling prescription by unitary transformation of $\mathbf{p}$, because for any differentiable function $f$ we have $e^{-i f(\mathbf{r}) \mathbf{P}_{Ta}} = \mathbf{p} + \nabla f(\mathbf{r})$. The gradient $\nabla f$ is a longitudinal field therefore we cannot have $\nabla f(\mathbf{r}) = -q \mathbf{A}(\mathbf{r})$ for all $\mathbf{r}$, because $\mathbf{A}_T(\mathbf{r})$ is non-vanishing. What is fundamental and completely general is the gauge-transformation $e^{i f(\mathbf{r})} [p - \mathbf{q}_A] e^{-i f(\mathbf{r})} = p - q[A + \nabla f(\mathbf{r})]$, which yields the result $R_{10} p R_{10}^\dagger = p - q A_\alpha$ as an approximate special case in which we let $f = \chi_0 - \chi_1$, and perform the EDA.

Turning our attention to the mechanical energy, Eq. (27) implies that this energy can be expressed in different gauges via gauge-transformation as

$$H_m(A_\alpha) = R_{10}^\dagger H_m(A_\alpha) R_{10}^\dagger,$$  \hfill (136)
which is an expression of the gauge-principle within the \(\alpha\)-gauge framework. However, as noted above (see also Sec. II), within the approximations made \(A_1 = (1 - \alpha)A_{(\alpha=1)} \equiv 0\), such that \(H_m(A_1)\) is actually independent of \(A\). Thus, for \(\alpha = 1\), Eq. (136) has the appearance of a unitary transformation applied to the free material Hamiltonian:

\[ H_m(A_\alpha) = R_{1\alpha} H_m R_{1\alpha}^\dagger \]  

(137)

where we have used that due to the EDA

\[ H_m(A_1) = H_m = \frac{p^2}{2m} + V(x). \]  

(138)

The transverse electromagnetic energy, \(H_{\text{ph},\alpha}\), from Eq. (28) can be written similarly as

\[ H_{\text{ph},\alpha'} = R_{\alpha\alpha'} H_{\text{ph},\alpha} R_{\alpha\alpha'}^\dagger \]  

(139)

and in particular,

\[ H_{\text{ph},\alpha} = R_{0\alpha} H_{\text{ph}} R_{0\alpha}^\dagger \]  

(140)

where

\[ H_{\text{ph}} = H_{\text{ph},0} = \frac{v}{2} \left((\Pi^2 + \omega^2 A^2)\right). \]  

(141)

Combining Eqs. (137) and (139) we see that within the simplified setting of a one-dimensional model in the EDA the Hamiltonian can be written in terms of unitary gauge-fixing transformations of the free Hamiltonians \(H_m\) and \(H_{\text{ph}}\) as

\[ H_\alpha = R_{1\alpha} H_m R_{1\alpha}^\dagger + R_{0\alpha} H_{\text{ph}} R_{0\alpha}^\dagger \]  

(142)

This is an approximate special case of the more general fundamental expression

\[ H_\alpha = R_{\alpha'} H_m(A_{\alpha'}) R_{\alpha'}^\dagger + R_{\alpha''\alpha} H_{\text{ph},\alpha''} R_{\alpha''\alpha}^\dagger \]  

(143)

which expresses that both \(H_m(A)\) and \(H_{\text{ph},\alpha}\) can be obtained as gauge-transformations of their counterparts in arbitrary gauges \(\alpha'\) and \(\alpha''\) respectively. This follows immediately from the definition of gauge-transformation given by Eqs. (27) and (28). Eq. (143) reduces to Eq. (142) when we choose \(\alpha' = 1\) and \(\alpha'' = 0\), and we make use of \(H_{\text{ph},0} = H_{\text{ph}}\) and \(H_m(A_1) = H_m\). This latter equality holds only because of the approximations and simplifying assumptions made, without which the derivation of \(H_m(A_\alpha)\) via unitary transformation of \(H_m\) is impossible.

### B. Material truncation

Let us now consider truncating the material Hilbert space. Since the canonical momentum \(p\) represents a different physical observable for each different value of \(\alpha\), the same is true of \(H_m\). Therefore, projecting onto a finite number of eigenstates of \(H_m\) is a gauge-dependent procedure. Eigenvalues of \(H_m\) are denoted \(\epsilon_n\). The projection \(P\) onto the first two levels \(|\epsilon^0\rangle, |\epsilon^1\rangle\) of \(H_m\) gives \(PH_mP = \omega_m \sigma^+ \sigma^- + \epsilon_0\) and \(Pq_x P = d \sigma^z\) where \(\sigma^+ = |\epsilon^1\rangle \langle \epsilon^0|, \sigma^- = |\epsilon^0\rangle \langle \epsilon^1|\) and \(\sigma^z = \sigma^+ + \sigma^-.\) The first transition energy is denoted \(\omega_m = \epsilon_1 - \epsilon_0\), and the transition dipole moment \(d = \langle \epsilon^0 | q_x | \epsilon^1\rangle\) is assumed to be real. More generally, one can define \(P\) as the projection onto any finite number of levels.

There are many ways to define two-level models using the projection \(P\). In general, a two-level truncation of \(H_\alpha\) is a \(P\)-dependent map \(M_P : H_\alpha \rightarrow M_P(H_\alpha)\), such that \(M_P(H_\alpha) : PH \rightarrow PH\) is an Hermitian operator on \(PH\). If, unlike the \(H_\alpha\), the \(M_P(H_\alpha)\) are not equivalent for different \(\alpha\), then truncation has broken the gauge-invariance of the theory. To obtain what we will refer to as the standard \(\alpha\)-gauge two-level model one replaces \(x\) and \(p\) with their projected counterparts \(P_xP\) and \(PP_P\) to obtain

\[ M_P(H_\alpha) = H_\alpha^P = PH m P + PH_{\text{ph}} P + V^\alpha(P_xP, PP_P) \]  

(144)

where \(V^\alpha(x,p) = H_\alpha - H_m - H_{\text{ph}}\) is the interaction Hamiltonian. The terminology “standard” is used because this definition of \(M_P\) is capable of yielding the standard quantum Rabi model (QRM) that is ubiquitous in light-matter physics. Specifically, a standard QRM is obtained by choosing \(\alpha = 1\) in Eq. (144). More generally, for distinct values of \(\alpha\) the Hamiltonians \(H_\alpha^P\) are not equivalent to each other [4, 5, 9]. This is because physically, \(P\) represents a different projection in each different gauge. The gauge-invariance of the theory has now been broken.

Of crucial importance when defining two-level models is recognition that for a Hermitian operator \(O\), projection \(P \neq I\), and non-linear function \(f\) we have

\[ Pf(O)P \neq f(POP). \]  

(145)

Thus, for a general material operator \(O(x,p)\) we have \(PO(x,p)P \neq O(P_xP, PP_P)\) with this inequality becoming an equality if and only if \(O\) is linear in \(x\) and \(p\) [4]. Since the interaction Hamiltonian \(H^P = H_m - H_{\text{ph}}\) contains a term \(vP_T^2/2\) quadratic in \(x\) for \(\alpha \neq 0\) we see that a different two-level model to that given by Eq. (144) can be defined simply as \(M_P(H_\alpha) = PH m \alpha\). To understand the difference between this two-level model and \(H_\alpha^P\) in Eq. (144) we note that by letting \(Q := I - P\) and making the approximation

\[ I \equiv P + Q \approx P \]  

(146)

within \(vP_T^2/2\), the two definitions become the same;

\[ P_x^2P \approx P_xP_xP = (P_xP)^2. \]  

(147)

The neglected difference, \(P_x^2P - P_xP_xP = P_xP_xP\), represents transitions inside the two-level subspace via intermediate states within the orthogonal complement.
One expects such contributions to be small for a sufficiently anharmonic material system. We note that in general, the neglect of such terms will become an increasingly poor approximation for increasingly nonlinear functions of \( x \). For example, writing \( P_x^2 P \approx P_x P \ldots P_x P \), in which \( Q \) has been neglected in between each factor of \( x \), will not be a valid for sufficiently large \( n \).

A third type of two-level model is obtained by including the quadratic term \( v P_x^2 \) within the material Hamiltonian giving an explicitly \( \alpha \)-dependent material Hamiltonian \( H^\alpha_m \) and projection \( P_\alpha \). The corresponding truncated Hamiltonian is \( M_P(H_\alpha) = P_\alpha H_\alpha P_\alpha = P_\alpha H^\alpha_m P_\alpha + P_\alpha H_{ph} P_\alpha + V(\rho P_\alpha^2, \rho P_\alpha) \) where the second equality holds because with inclusion of the quadratic function of \( x \) within \( H^\alpha_m \) the corresponding interaction \( V_\alpha = V_\alpha - v P_x^2 \omega^2 / 2 \) is linear in \( x \) and \( p \). This definition of truncation possesses the complication that the material eigenenergies of \( H^\alpha_m \) are now \( \alpha \)-dependent.

Clearly there are many ways of defining two-level models. Two further methods have been proposed in Ref. [7] (see also Ref. [13]). Both methods require the EDA and involve deriving two-level models from the free theory by replacing the unitary transformation \( R_\alpha \) in Eq. (142) with a two-level model counterpart. Due to Eq. (145) there are two different two-level model versions of \( R_\alpha \) within \( H \rightarrow H \), which are defined as

\[
G_{\alpha \alpha'} = P R_{\alpha \alpha'} P = P \exp[i(q_\alpha - q_{\alpha'})x_A] P \quad (148)
\]

\[
T_{\alpha \alpha'} = \exp[i(q_\alpha - q_{\alpha'})P_x P A] \neq G_{\alpha \alpha'} \quad (149)
\]

where the final inequality holds because as noted above \( e^{P_x P} \neq P e^{P_x} \) [cf. Eq. (145)]. Moreover, we cannot expect this inequality to become an approximate equality even for highly anharmonic material systems. The first of the above transformations \( G_{\alpha \alpha'} \) is not unitary. However, it does implement a gauge change in a projected operator because if we let \( POP = F(p) \), where \( O \) is arbitrary, then we have

\[
G_{\alpha \alpha'} F(p) G_{\alpha \alpha'} = PF(p - (\alpha - \alpha')q_A), \quad (150)
\]

which follows immediately from Eq. (131). In words, \( G_{\alpha \alpha'} \) implements a gauge-transformation within a projected operator and then re-projects the result. By replacing \( R_{\alpha \alpha'} \) in Eq. (142) [or (143)] with \( G_{\alpha \alpha'} \) one obtains a new kind of two-level model

\[
\tilde{H}_\alpha^2 = G_{\alpha \alpha} H_m G_{\alpha \alpha}^* + G_{\alpha \alpha} H_{ph} G_{\alpha \alpha}^* \quad (151)
\]

These models are not equivalent for different \( \alpha \).

The other two-level model transformation \( T_{\alpha \alpha'} \) which is given in Eq. (149) is clearly unitary (unlike \( G_{\alpha \alpha'} \)), but it does not implement a gauge change even in a projected operator \( F(p) = POP \):

\[
T_{\alpha \alpha'} F(p) T_{\alpha \alpha'} \neq PF(p - (\alpha - \alpha')q_A) \quad (152)
\]

Indeed, a two-level model unitary transformation cannot implement the minimal-coupling replacement \( p \rightarrow q \cdot \alpha \), because the required operator algebra cannot be supported by the truncated space. By replacing \( R_{\alpha \alpha'} \) in Eq. (142) [or (143)] with \( T_{\alpha \alpha'} \) one obtains the two-level models

\[
h_\alpha^2(\alpha) = T_{\alpha \alpha} P H_m P T_{\alpha \alpha}^* + T_{\alpha \alpha} P H_{ph} P T_{\alpha \alpha}^* = T_{\alpha \alpha} H_{\alpha}^2 T_{\alpha \alpha}^* \quad (153)
\]

where the second equality shows that these models are equivalent to the standard multipolar-gauge QRM \( H_\alpha^2 \). In particular, \( h_\alpha^2(1) = H_\alpha^2 \). Unlike the transformations \( G_{\alpha \alpha'} \) the \( T_{\alpha \alpha'} \) do not possess the defining properties of a gauge transformation (see Sec. III E). The difference between the model \( h_\alpha^2(\alpha) \) and the standard model \( H_\alpha^2 \) in Eq. (144) stems entirely from the first term \( T_{\alpha \alpha} P H_m P T_{\alpha \alpha}^* \) in Eq. (153). Thus, \( h_\alpha^2(1) = H_\alpha^2 \) is the standard multipolar-gauge QRM. In Sec. III C we will see that the equivalent models \( h_\alpha(\alpha)^2 \) all belong to the multipolar-gauge and are a special case of a more general result, \( h_\alpha^2(\alpha) \). Here \( \alpha \) selects the gauge within which truncation is performed and \( \alpha' \) parametrizes a rotation within this truncation. Importantly, any two models resulting from truncation in different gauges are not equivalent to each other.

Although it is clear that \( T_{\alpha \alpha'} \neq G_{\alpha \alpha'} \) it is instructive to consider how the associated two-level models in Eqs. (151) and (153) differ. We therefore express \( G_{\alpha \alpha} \) in the form

\[
G_{10} = P \exp[i(\sigma^\alpha + [P_x Q + Q_x P + Q_x Q]/\tilde{\sigma})(\alpha^\dagger + \alpha)] P \quad (154)
\]

where \( \tilde{\sigma} = d/\sqrt{2 \omega v} \) is a dimensionless coupling parameter, \( \tilde{x} = \langle e^0| x | e^0 \rangle = d/q \) and \( \sigma^\alpha = P_x P/\tilde{x} \). If we assume that \( P_x Q \ll P_x P \) such that terms \( P_x Q \) and \( Q_x P \) can be neglected in the exponent of \( R_{10} \) then we obtain

\[
G_{10} \approx P \exp[i(\sigma^\alpha + Q_x Q/\tilde{x})(\alpha^\dagger + \alpha)] P \quad (155)
\]

where we have used \( PQ = 0 = QP \). However, as already noted, such a naive approximation cannot be justified, even for a sufficiently anharmonic material system. To see this note that by employing the approximation and following exactly the same steps as above one obtains

\[
T_{\alpha \alpha'} \approx P R_{\alpha \alpha'} \quad (156)
\]

This exemplifies the importance of inequality (145).
The approximate equality $\mathcal{T}_{\alpha \alpha'} \approx \mathcal{G}_{\alpha \alpha'}$ does result if the exponentials on both sides are expanded to linear order in $q$. In this case the two-level models $\hat{H}_2^\alpha$ are then the same as the models $\hat{h}_2^\alpha(\alpha)$ and they must be equivalent to each other for different $\alpha$. However, a first order expansion of the model $\hat{h}_2^\alpha(\alpha)$ simply gives back the standard two-level model $H_2^\alpha$ but with quadratic terms neglected. It follows that in the weak-coupling regime all two-level models are the same $H_2^\alpha = \hat{h}_2^\alpha(\alpha) = H_2^\alpha$. This is the only regime in which such an equivalence can generally be obtained. As the coupling-strength increases the first order expansion in $q$ becomes progressively worse, so $\mathcal{T}_{\alpha \alpha'}$ and $\mathcal{G}_{\alpha \alpha'}$ become progressively different. Thus, if a particular model $H_2^\alpha$ were found to be accurate for some particular observable in some particular situation, then as the coupling increases any other model $H_2^\alpha$, $\alpha_2 \neq \alpha_1$ can be expected to become progressively less accurate by comparison. The relative optimality of different two-level models is discussed in Sec. III F.

C. Phase-invariance with respect to truncated position

Supplementary Note 1 of Ref. [7] provides an alternative derivation of the multipolar equivalence class $\{\hat{h}_2^\alpha(\alpha')\}$ as resulting from the imposition of a phase-invariance principle defined using the truncated position operator $x_P := PxP$. More generally, this principle can be applied in any gauge $\alpha$ and it yields the equivalence class $\{\hat{h}_2^\alpha(\alpha')\}$.

In the first quantised-setting the gauge-principle asserts that the mechanical energy $\mathcal{H}_m(A_\alpha)$ in Eq. (134) satisfies local phase-invariance (gauge-invariance) in the form

$$\langle \psi | \mathcal{H}_m(A_\alpha) | \psi \rangle = \langle \psi' | \mathcal{H}_m(A'_\alpha) | \psi' \rangle$$

where $|\psi'\rangle = e^{i\chi_\alpha} |\psi\rangle$ and $A'_\alpha = A_\alpha + \nabla \chi$. In particular, the equality $\langle \psi_\alpha | \mathcal{H}_m(A_\alpha) | \psi_\alpha \rangle = \langle \psi_\alpha' | \mathcal{H}_m(A'_\alpha) | \psi_\alpha' \rangle$ in which $|\psi_\alpha'\rangle = R_{\alpha \alpha'} |\psi_\alpha\rangle$, expresses gauge-invariance within the $\alpha$-gauge framework and is a special case of Eq. (156) obtained by letting $\chi = \chi_\alpha - \chi_\alpha$.

To define the class $\{\hat{h}_2^\alpha(\alpha)\}$, the gauge-fixing transformation $R_{1 \alpha}$ was replaced with $T_{\alpha \alpha}$ in Eq. (137) and the multipolar-gauge mechanical energy $\mathcal{H}_m(A_1) = H_m$ in Eq. (138) was replaced with its projection $\mathcal{P}\mathcal{H}_m(A_1) P$. More generally however, Eqs. (137) and (138) are special cases of Eqs. (136) and (134) respectively. If we replace $R_{\alpha \alpha'}$ with $T_{\alpha \alpha}$ and $\mathcal{H}_m(A_\alpha)$ with $\mathcal{H}_m^2(A_\alpha) := \mathcal{P}\mathcal{H}_m(A_\alpha) P$ on the right-hand-side of Eq. (136), then we obtain a truncated $\alpha'$-“gauge” mechanical energy analogous to that in Eq. (136);

$$\mathcal{H}_{m,\alpha'}^2(A_{\alpha'}) := \mathcal{T}_{\alpha \alpha'} \mathcal{H}_m^2(A_\alpha) \mathcal{T}_{\alpha \alpha'}^{-1}$$

expressed as a rotation of the $\alpha$-gauge mechanical energy after two-level truncation. This truncated energy satisfies a form of phase-invariance analogous to Eq. (156) but defined with respect to the truncated position operator $x_P := PxP$. The phase transformation is defined by

$$U_{xp} = e^{i\chi(x_P)} = e^{i\beta e^{id\Lambda x}}$$

where $\beta$ and $\Lambda$ are constants depending on the choice of function $\chi$. The global phase $e^{i\beta}$ can be ignored. Letting $|\psi_2\rangle = P |\psi\rangle$ denote an arbitrary truncated state we have

$$\langle \psi_2 | \mathcal{H}_{m,\alpha}^2(A_{\alpha'}) | \psi_2 \rangle = \langle \psi_2' | \mathcal{H}_{m,\alpha}^2(A'_{\alpha'}) | \psi_2' \rangle$$

where $A_{\alpha'} = A_{\alpha'} + \partial_{x_P} \chi(x_P) = A_{\alpha'} + \Lambda$ and $|\psi_2\rangle = U_{xp} |\psi_2\rangle$. Thus, we see that $\mathcal{H}_{m,\alpha}^2(A_{\alpha'})$ is the mechanical energy of the $\alpha'$-“gauge” where here the term “gauge” does not possess the same meaning as in the non-truncated theory but instead refers to $x_P$-phase-invariance within the $\alpha$-gauge truncated mechanical energy. Subsequently, a “gauge”-transformation of $A_{\alpha'}$ under this principle is $A_{\alpha'}' = A_{\alpha'} + \Lambda$.

To obtain the complete $\alpha'$-dependent Hamiltonian one adds the transverse electromagnetic energy, $\mathcal{H}_{ph,\alpha'}$, defined in Eq. (135), to the mechanical energy. This gives the total energy. Following the standard method of obtaining two-level models we note that $E_T = -\Pi - \alpha'd\sigma^2/v = -\Pi - P_{\alpha'}$, is the transverse electric field within the two-level truncation, and we thereby define the transverse electromagnetic energy $\mathcal{H}_{ph,\alpha'}^2$ as

$$\mathcal{H}_{ph,\alpha'}^2 := \frac{v}{2} \left[ \left( \Pi + \alpha'd\sigma^2/v \right)^2 + \alpha^2 A^2 \right]$$

$$= \mathcal{T}_{\alpha \alpha'} \mathcal{H}_{ph,\alpha}^2 \mathcal{T}_{\alpha \alpha'} = \mathcal{T}_{\alpha \alpha'} \mathcal{H}_m^2 \mathcal{T}_{\alpha \alpha'}^{-1}. \quad (160)$$

The second equality in Eq. (160) follows from the fact that unlike when acting on $p$, the transformation $\mathcal{T}_{\alpha \alpha'}$ has the same effect as a gauge-transformation when acting on $\Pi$, because truncation does not alter the algebra of photonic operators. Combining Eqs. (157) and (160) we may now define the full $\alpha'$-dependent two-level model as the total energy

$$\hat{h}_2^\alpha(\alpha') = \mathcal{H}_{m,\alpha}^2(A_{\alpha'}) + \mathcal{H}_{ph,\alpha'}^2 = \mathcal{T}_{\alpha \alpha'} \mathcal{H}_m^2 \mathcal{T}_{\alpha \alpha'}^{-1}. \quad (161)$$

Thus, the equivalence class $\{\hat{h}_2^\alpha(\alpha')\}$ can be obtained as the class of Hamiltonians satisfying $x_P$-phase-invariance after truncation within the $\alpha$-gauge. The particular class $\{\hat{h}_2^\alpha(\alpha)\}$ results if the $x_P$-phase-invariance principle is applied within the multipolar-gauge. Such application has the appearance of an application to the free theory only due to approximations that have implied that $A_1 \equiv 0$ so that $p - qA_1 = p$, and therefore that $\mathcal{H}_m(A_\alpha) \equiv R_{1 \alpha} \mathcal{H}_m(A_1) R_{1 \alpha}^\dagger = R_{1 \alpha} \mathcal{H}_m R_{1 \alpha}^\dagger$.

D. Relating models belonging to different equivalence classes

Further insight into the nature of the models $\hat{h}_2^\alpha(\alpha')$ may be obtained by asking how any given standard two-level model must be modified in order that it coincides
with the standard two-level model found using a different gauge. For example, let us consider the term $q^2 \mathbf{A}^2 / 2m$ of the Coulomb-gauge Hamiltonian. The coefficient $q^2 / 2m$ is related to the material dipole moment and transition frequencies by the TRK sum rule as

$$\sum_n \omega_n d_{1n}^i d_{1n}^j = i \frac{e^2}{2m} \langle c^i | [p_i, r_j] | c^j \rangle = \delta_{ij} \frac{q^2}{2m}.$$  \tag{162}$$

This result rests directly on the CCR algebra $[r_i, p_j] = i \delta_{ij}$ which as already noted, can only be supported in an infinite-dimensional Hilbert space. Eq. (162) is independent of the level $l$ appearing on the left-hand-side. However, if on the left-hand-side we restrict ourselves to two levels $n, l = 0, 1$ with energy difference $\omega_m$, then for $l = 1$ Eq. (162) reads

$$\sum_n \omega_n d_{1n}^i d_{1n}^j = -\omega_m d_{10}^i d_{10}^j$$  \tag{163}$$

wheras for $l = 0$ Eq. (162) reads

$$\sum_n \omega_n d_{10}^i d_{10}^j = +\omega_m d_{10}^i d_{10}^j.$$  \tag{164}$$

The result obtained now clearly depends on whether $l$ is the ground or excited state. As first noted in Refs. [4, 71], if one takes the two-level projection of the Coulomb-gauge self-energy term, namely, $q^2 \mathbf{A}^2 (|0\rangle \langle 0| + |1\rangle \langle 1|)/2m$, and one applies Eqs. (163) and (164) to the excited state projection $q^2 |1\rangle \langle 1|/2m$ and the ground state projection $q^2 |0\rangle \langle 0|/2m$ respectively, then one arrives at the following modified term, which now constitutes a non-trivial light-matter interaction:

$$\frac{q^2}{2m} \mathbf{A}^2 \rightarrow -\omega_m (\mathbf{d} \cdot \mathbf{A})^2 \sigma^z$$  \tag{165}$$

where $\mathbf{d} := \mathbf{d}_{10}$ and $\sigma^z = |1\rangle \langle 1| - |0\rangle \langle 0|$. As noted in Ref. [7] the modification (165) is ad hoc. It results in a model that no longer has the interaction of the Coulomb-gauge. However, in order $q^2$ the model obtained does coincide with the multipolar-gauge model $h_1^2(0)$ [7]. In this sense the truncated “gauge”-principle can reveal what ad hoc non-unitary modifications are required in order to relate non-equivalent truncated theories.

As already noted, at order $q$ all two-level models are equivalent without any modification. At order $q^2$, forcing equivalence requires a non-unitary modification of at least one of the models involved, such that it no longer represents the gauge within which it was derived. As the coupling-strength increases, increasingly drastic non-unitary modifications will be needed to transform a given model into one that belongs to a different equivalence class. This perspective is another way to understand the increasing difference with increasing coupling strength, between the gauge transformations $PR_{\alpha\alpha'}$ or $PR_{\alpha\alpha'}P$ and the rotation $T_{\alpha\alpha'}$.

### E. Misidentification of gauge transformations

It has been argued within the literature that the transformation $T_{\alpha\alpha'}$ constitutes a two-level model gauge transformation and that since $T_{\alpha\alpha}$ is unitary, this resolves any gauge non-invariance due to truncation [7, 13]. However, the inequality (152) states that $T_{\alpha\alpha}$ does not implement a gauge change when acting on (projected) functions of $p$. The action of $T_{\alpha\alpha'}$ coincides with that of the gauge transformation $R_{\alpha\alpha'}$ followed by projection $P$, only when acting on operators that commute with $R_{\alpha\alpha'}$ (functions of $x$ and $A$) and linear functions of $\Pi$, for which it is clear that

$$PR_{\alpha\alpha'} \Pi R_{\alpha\alpha'}^\dagger P = T_{\alpha\alpha'} \Pi T_{\alpha\alpha'}^\dagger.$$  \tag{166}$$

As we have shown (see also Ref. [12]) the invariance of the models related by $T_{\alpha\alpha'}$ is $xP$-phase invariance rather than gauge-invariance.

Different gauges constitute different associations between operators and observables and therefore possess different corresponding decompositions of the light-matter composite into light and matter subsystems (see Sec. II.K). A two-level model unitary operator cannot preserve these associations in general. The misidentification of $T_{\alpha\alpha}$ as a gauge transformation and of $h_1^2(0)$ as a Coulomb-gauge model, as in Refs. [7, 13], will produce incorrect results when dealing with observables represented by functions of $p$. Consider, for example, the total momentum

$$\mathbf{K} := m\mathbf{r} + K_{\text{long}} + K_{\text{trans}},$$  \tag{167}$$

which is a fundamental conserved quantity. Here $K_{\text{trans}} = \int d^3x (\mathbf{E}_T \times \mathbf{B} - \mathbf{B} \times \mathbf{E}_T)/2$ and $K_{\text{long}}$ is defined in Eq. (87). Since in the Coulomb-gauge $\mathbf{p} = m\mathbf{r} + q\mathbf{A}_T(r)$, it follows from Eq. (87) that $K_{\text{m, long}} := m\mathbf{r} + K_{\text{long}} = \mathbf{p}$. The two-level truncation of this observable is $P\mathbf{p}P = (m/q)\omega_m \sigma^y$ where $\omega_m = e^2 - e^0$, $\mathbf{d} = q |1\rangle \langle 1|$ and $\sigma^y = -i(\sigma^+ \sigma^-) + \sigma^z$ the usual raising and lowering operators for the lowest two material levels. The energy corresponding to $K_{\text{m, long}}$ is that of an atom dressed by its electrostatic field:

$$E_{\text{m, long}} := \frac{K_{\text{m, long}}^2}{2m} + V(r),$$  \tag{168}$$

which is represented in the Coulomb-gauge by the material bare-energy operator $H_m = \mathbf{p}^2/(2m) + V(r)$.

In the multipolar-gauge, the observables $K_{\text{m, long}}$ and $E_{\text{m, long}}$ for a dipole are represented by the operators

$$K_{\text{m, long}} = R_{01} \mathbf{p} R_{01}^\dagger = \mathbf{p} + q\mathbf{A}_T(0),$$  \tag{169}$$

$$E_{\text{m, long}} = R_{01} H_m R_{01}^\dagger = \frac{1}{2m} [(\mathbf{p} + q\mathbf{A}_T(0))^2 + V(r)] = H_m + \frac{q}{m} \mathbf{p} \cdot \mathbf{A}_T(0) + \frac{q^2}{2m} \mathbf{A}_T(0)^2.$$  \tag{170}$$
within the multipolar-gauge are
\[ K_{m,\text{long}} = \frac{m}{q} \omega_m d \sigma^y + q A_T(0), \]  
\[ E_{m,\text{long}} = \omega_m \sigma^+ \sigma^- + e^0 - \omega_m d \cdot A_T(0) \sigma^y + \frac{q^2}{2m} A_T(0)^2. \]

This is the same definition of truncation that yields the standard multipolar QRM $H^1$, which is equivalent to the model $h^1(0) = T_{10} H^1_T T_{10}^\dagger$ where \([7, 13]\)

\[ T_{10} = \exp[iq \mathbf{r} \mathbf{P} \cdot A_T(0)] = \exp[\mathbf{d} \cdot A_T(0) \sigma^z]. \]

Note that since for the present discussion there is no need to restrict the spatial dimension or the number of radiation modes, we have not done so in the above equations.

If $h^1(0)$ is a Coulomb-gauge model then the observables $K_{m,\text{long}}$ and $E_{m,\text{long}}$ must be represented within this “gauge” by $K_{m,\text{long}} = (m/q) \omega_m d \sigma^y$ and $E_{m,l} = \omega_m \sigma^+ \sigma^- + e^0$. If $T_{10}$ is a gauge transformation then within the multipolar-gauge truncation these observables associated with the Coulomb “gauge” to the multipolar-gauge; 
\[ K_{m,\text{long}} = (m/q) \omega_m d T_{10} \sigma^y T_{10}^\dagger, \]
\[ E_{m,\text{long}} = \omega_m T_{10} \sigma^+ \sigma^- T_{10}^\dagger + e^0, \]

which are different to Eqs. (170) and (171). Hence we have arrived at a contradiction. Specifically, under the truncating map $M_P$ yielding the standard QRM $H^1_T$, which is equivalent to $h^1(0)$, the associations between operators and observables within the multipolar-gauge truncation contradicts the associations implied if $h^1(0)$ is identified as a Coulomb-gauge model.

In any quantum theory a unitary rotation can be used to generate an equivalent representation of a given observable. This fact is trivial. However, in a truncated theory, the association between an operator and an observable after a unitary rotation will not in general coincide with that implied by identifying the rotated frame as a different gauge. This is because a gauge constitutes a particular association between operators and observables within the non-truncated theory, yet truncation does not preserve the algebra of material operators. Conversely, treating the truncated theory’s rotated frame as a different gauge, i.e., using the associations between operators and observables that define this gauge, will generally result in the incorrect operator representation of a given observable within the truncated theory.

In order to correctly identify within a truncated theory, alternative unitary representations of a physical observable $O$ represented by operator $O$, first an accurate truncation, $O^2$, must be found. This can then be taken to define the correct association $O^2 \leftrightarrow O$ within the truncated theory. Subsequently, any two level model unitary rotation, $U^2$, may be used to generate an equivalent representation of $O$ as $U^2 O^2( U^2)^\dagger$. The rotation $T_{10}$ is simply an arbitrary example of such a rotation. The important task is that of determining initially an accurate truncation for the given observable property. The subsequent possibility of two-level unitary rotation is trivial. The optimality of competing truncations is discussed below.

### F. Optimality of truncations

Having reviewed the various methods of obtaining two-level models and discussed how they are non-unitarily related, we briefly discuss which two-level models are known to be accurate in which situations. Subsequently we discuss the importance of two-level model predictions for gauge-ambiguities.

The truncation to two material levels should be expected to offer a robust approximation of the more complete theory when the material system is sufficiently anharmonic that the orthogonal subspace $QH$ is sufficiently well separated from $PH$, where $PH \oplus QH = H$ is the full Hilbert space. Such regimes may or may not be of experimental importance when considering specific systems and implementations of light-matter physics models.

Let us first suppose we have a highly anharmonic system at arbitrary coupling strength and only a single radiation mode. The Coulomb-gauge coupling involves the canonical momentum $p$, which possesses matrix elements in the material basis $\{x^n\}$ that scale with material transition frequencies as
\[ q \mathbf{p}_{\text{mat}} = im \omega_m d n. \]

As first explained in Ref. [9] transitions to higher states are not suppressed within the Coulomb gauge, because the increasing energy gap is compensated by an increasing coupling matrix element. In contrast, the multipolar coupling involves only the dipole moment. Therefore, for sufficiently strong coupling where two-level models are not equivalent, the Coulomb-gauge truncation will generally perform poorly in comparison to the multipolar-gauge truncation as a general approximation of the non-truncated theory. These points were also elaborated in Ref. [4] via a Schriefer-Wolf-type analysis. As an illustrative example we take a double-well dipole with potential $V(\theta, \phi) = -\theta^2/2 + \phi^4/4$ where $\theta$ and $\phi$ control the shape of the double-well \([6, 7, 9]\). The material Hamiltonian is therefore [9]
\[ H_m^0 = \frac{\mathcal{E}}{2} \left( -\partial^2 + \beta \xi^2 + \xi^4 \right) \]

where we have defined the dimensionless variable $\xi = r/r_0$ with $r_0 = (1/[m \omega])^{1/6}$, along with $\mathcal{E} = 1/(m r_0^3)$ and $\beta = \theta m r_0^4$. We first consider the case of resonance $\delta = \omega/\omega_m = 1$ together with a high anharmonicity $\mu = (\omega_2 - \omega_1)/\omega_m$ of $\mu = 70$. We compare the unique spectrum of the non-truncated Hamiltonian $H_0$, with the different approximations given by the spectra of the standard multipolar and Coulomb-gauge quantum Rabi models (QRMs) $H^1_T$ and $H^2_T$, and also with the non-standard...
generally breaking down for higher levels \[4\]. This is il-
sentation than the multipolar QRM, despite truncation for low energy states, and offer a more accurate repre-
terial systems with low anharmonicity remain accurate
\(\alpha\) ground state; \(\mu := (\omega_2 - \omega_m)/\omega_m = 70\) and resonance \(\delta := \omega/\omega_m = 1\). The mul-
tipolar gauge QRM is generally accurate in this regime, in
the sense that one must go to very high energy levels before
discrepancies with the exact spectrum are found. The two
Coulomb-gauge two-level models \(H_\alpha^{\text{JC}}\) and \(H_\alpha^{\text{IC}}\) are generally in-
accurate, and are qualitatively very similar.

\[
\begin{align*}
E - G/
\hline
0 & 1 \hline
0 & 1 \hline
\end{align*}
\]

FIG. 2: The transition spectra (relative to the ground en-
ergy \(G\)) of two-level models \(H_\alpha^{\text{JC}}\) and \(H_\alpha^{\text{IC}}\), are compared with the exact transition
spectrum, assuming a material anharmonicity of \(\mu \approx 3\) and resonance \(\delta = 1\). The \(\alpha\)JC-gauge two-level model can be more accurate
than the multipolar-gauge QRM in the ultrastrong-coupling
regime.

Coulomb-gauge model \(\tilde{H}_\alpha^2\) defined by Eq. (151). We note
that for each \(\alpha\) the standard two-level model \(H_\alpha^2\) can be
selected as the representative of its unitary equivalence
class \(\{h_\alpha^2(\alpha')\}\) without loss of generality. As shown in
Fig. 2, the multipolar-gauge QRM \(H_\alpha^2\) is very accurate
for predicting transition spectra in this regime while the
Coulomb-gauge models \(H_\alpha^{\text{JC}}\) and \(H_\alpha^{\text{IC}}\) are qualitatively sim-
ilar and very inaccurate for strong enough couplings.

Although two-level truncation will obviously break-
down as a general approximation for sufficiently har-
monic material systems, in Ref. [4] a gauge denoted \(\alpha\)JC
was identified for which the two-level truncation of a
material harmonic oscillator nevertheless yields the ex-
act ground state; \(P|G_{\alpha\text{JC}}\rangle = |G_{\alpha\text{JC}}\rangle\). Full details of this
case are given in Sec. IV B 1. For this reason, there exist
gauges \(\alpha \neq 1\) in which the two-level truncation of ma-
terial systems with low anharmonicity remain accurate
for low energy states, and offer a more accurate repre-
sentation than the multipolar QRM, despite truncation
generally breaking down for higher levels [4]. This is il-
illustrated in Fig. 3 using the double-well dipole example
and a material anharmonicity of \(\mu \approx 3\). The existence
of such gauges and the accuracy of two-level truncation
for low energy properties therein, is of importance for
understanding gauge-ambiguities in the USC regime, as
will be discussed below in Sec. III G.

When more radiation modes are considered the opti-
-\mal \(\alpha\) for truncation may often be shifted away
from the multipolar-gauge \(\alpha = 1\) towards the Coulomb-
gauge \(\alpha = 0\) [8]. While the multipolar linear interaction
component scales as \(\sqrt{\delta}\), the Coulomb-gauge linear inter-
action instead scales as \(1/\sqrt{\delta}\). In the same way that the
effects of additional material levels are more pronounced
in the Coulomb-gauge, the introduction of more radi-
ation modes causes the multipolar gauge truncation to
\[\begin{align*}
E - G/
\hline
0 & 1 \hline
0 & 1 \hline
\end{align*}
\]

FIG. 3: The first transition energies of the two-level models
\(H_\alpha^2\) and \(H_\alpha^{\text{JC}}\), are compared with the exact transition energy,
assuming a material anharmonicity of \(\mu \approx 3\) and resonance
\(\delta = 1\). The \(\alpha\)JC-gauge two-level model can be more accurate
than the multipolar-gauge QRM in the ultrastrong-coupling
regime.

G. Gauge-ambiguities versus gauge non-invariance

Gauge non-invariance and gauge-ambiguities are not
synonymous. Gauge non-invariance can only result from
approximations and can therefore be avoided by avoid-
ing the offending approximation. In particular, the opti-
mality of a truncation is a separate consideration to
the physically motivated question of which gauge pro-
provides the most operationally relevant definitions of the quantum subsystems in a given experiment. The term gauge-ambiguities first used in the context of ultrastrong coupling (USC) light-matter physics in Ref. [4] refers to ambiguities that result from the inherent gauge-relativity of QED subsystems, a feature of QED that is independent of model approximations.

The onset of USC has often been identified through a departure from Jaynes-Cummings physics, due to the breakdown of the rotating-wave approximation (RWA). In the USC regime the qualitative low energy physics of the Jaynes-Cummings model (JCM) is markedly different to that of the quantum Rabi model (QRM). For example, unlike the quantum Rabi model the Jaynes-Cummings model predicts no ground state entanglement and no ground state photon population for all coupling strengths. The contrary predictions of the QRM have previously been regarded as definitive of ultrastrong-coupling phenomenology. However, Ref. [4] shows that there exists a gauge choice that yields a Jaynes-Cummings model without performing the RWA. The corresponding gauge-parameter \( \alpha_{JC} \) varies with the coupling and detuning parameters of the theory, but this is certainly permissible, it simply amounts to choosing a non-constant gauge-function (cf. Sec II G).

Independent of its robustness as an approximation, material truncation may be a useful tool. For a material harmonic oscillator two-level truncation is essentially as poor a general approximation as it can ever be, yet for this system there nevertheless exists a gauge \( \alpha_{JC} \) for which the ground state of the truncated model is \textit{exact} (cf. Sec. IV B 1). Ref. [4] exemplifies an experimentally realistic regime of a fluxonium LC-oscillator system with anharmonicity \( \mu \approx 3 \) and resonance \( \delta = 1 \). The number of JC-gauge photons is much lower than the number of flux-gauge photons. Appreciable JC-gauge photon population only occurs for very large couplings approaching the deep-strong limit \( \eta = 1 \).

\[ \text{FIG. 4: The exact ground state average numbers of flux-gauge and JC-gauge photons with coupling strength } \eta \text{ for a fluxonium system assuming an anharmonicity of } \mu \approx 3 \text{ and resonance } \delta = 1. \text{ The number of JC-gauge photons is much lower than the number of flux-gauge photons. Appreciable JC-gauge photon population only occurs for very large couplings approaching the deep-strong limit } \eta = 1. \]

\[ \text{FIG. 5: The exact ground state average numbers of multipolar-gauge, Coulomb-gauge, and JC-gauge photons for a double-well dipolar system assuming an anharmonicity of } \mu \approx 70 \text{ and resonance } \delta = 1. \text{ The number of JC-gauge photons is only appreciable well into the USC regime } \eta > 1/2. \]

\[ \text{IV. TIME-DEPENDENT INTERACTIONS AND ADIABATIC SWITCHING} \]

Time-dependent interactions arise in a number of contexts in light-matter physics. Herein, the notion of a process in which material charges exchange photons, is elementary. The concept arises from scattering theory wherein the interaction is adiabatically switched on and off over an infinite duration. Such an idealisation may not however, be applicable in extreme light-matter interaction regimes. We begin by discussing scattering theory, explaining why subsystem gauge-relativity can be completely ignored in calculating the S-matrix. We then directly demonstrate that conventional quantum optical approximations mimic the S-matrix, such that subsystem gauge-relativity is only eliminated after a sufficient
number of these approximations are performed. Only then does an “atom” defined as a quantum subsystem, become an ostensibly unique concept. We finally discuss non-adiabatic switching of ultrastrong couplings whereby subsystem gauge-relativity becomes important.

A. Adiabatic switching and a unique invariance property of the S-matrix

As explained in Secs. IIK-II M, the task we are faced with is the determination of which gauge-invariant subsystem definitions are relevant in which physical situations. However, if the S-matrix is applicable in providing all physical predictions then we are able to completely ignore this question. The QED S-matrix provides probability amplitudes for transitions between unperturbed states yet as explained below, subsystems become ostensibly unique within scattering theory. Feynman diagrams can be used as a mnemonic when calculating the terms in a perturbative expansion of the Hamiltonian resolvent used to define the S-matrix. This gives rise to the notions of “real” and “virtual” processes. The S-matrix is the primary source of predictions in high-energy and particle physics, and it possesses unique properties. We briefly review the definition of the S-matrix and discuss its limitations.

Let us begin by considering the matrix elements of the evolution operator in the unperturbed basis. The α-gauge Hamiltonian can be partitioned as \( H_\alpha = h + V^\alpha \) where \( h = H_m + H_{ph} \) is the unperturbed Hamiltonian and \( V^\alpha \) is the interaction. The unperturbed energy eigenvalues and eigenvectors are defined by \( h |e^n\rangle = \epsilon^n |e^n\rangle \). The unperturbed vectors \( \{|e^n\rangle\} \) are each a tensor product of an eigenvector of \( H_m \) and an eigenvector of \( H_{ph} \) (photon number state). The state represented by the vector \( |e^n\rangle \) in the gauge \( \alpha \) is represented by the vector \( |e^m\rangle = R_{\alpha\alpha'}|e^n\rangle \) in the gauge \( \alpha' \), therefore the bare eigenvectors of \( h \) represent different physical states in each gauge (subsystems are gauge-relative).

The evolution operator generated by \( H_\alpha \) between times \( t_i \) and \( t_f \) is denoted \( U_\alpha(t_i,t_f) \). Evolutions in different gauges are related by \( U_{\alpha'}(t_i,t_f) = R_{\alpha\alpha'}U_\alpha(t_i,t_f)R_{\alpha\alpha'}^\dagger \). It follows that the evolution operator matrix elements are gauge-invariant:

\[
(\epsilon^n|U_\alpha(t_i,t_f)|\epsilon^m) = (\epsilon^m|U_{\alpha'}(t_i,t_f)|\epsilon^m) .
\]  

(177)

It is equally clear that for \( \alpha \neq \alpha' \) we have

\[
(\epsilon^n|U_{\alpha'}(t_i,t_f)|\epsilon^m) \neq (\epsilon^n|U_\alpha(t_i,t_f)|\epsilon^m) .
\]

(178)

Inequality (178) simply exemplifies the expected result that an eigenvector of \( h \) represents a different physical state in each different gauge.

However, in scattering theory it is assumed that \( V^\alpha = 0 \) in the remote past and distant future \( t = \pm \infty \), such that at these times \( H = h \), so the unperturbed energy eigenvectors uniquely represent the total energy eigenstates. It is then assumed that the interaction is switched-on and -off adiabatically between \( t = \pm \infty \). Subsequently, the S-matrix is formally defined by [24, 73]

\[
S_{nm} = \lim_{t \to \infty} \langle \epsilon^n|U_{\alpha I}(-t,t)|\epsilon^m\rangle
\]

(179)

where \( U_{\alpha I} \) denotes the corresponding evolution operator in the interaction picture defined by \( h \). In contrast to inequality (178), the S-matrix possesses the remarkable property that it is independent of \( \alpha \) despite being defined in terms of the same unperturbed vectors for each \( \alpha \). In calculating \( S_{nm} \), we do not have to transform the eigenvectors of \( h \) in order to ensure that we are using the same physical state in each gauge, as in Eq. (177). In other words, “photons” and “material” excitations represented by the eigenstates of \( h \) become ostensibly unique in scattering theory, so we do not have to confront the question of which subsystem definitions are the most relevant.

A general proof of this unique invariance property of the S-matrix has been given for non-relativistic QED by Woolley [35, 74]. Essential for the proof is that the unperturbed operator \( h \) is kept the same in each gauge. The S-matrix can also be expressed in the form [35, 74, 75]

\[
S_{nm} = \delta_{nm} - 2\pi i T_{nm}\delta(\epsilon_n - \epsilon_m)
\]

(180)

where \( T \) is called the transition matrix whose elements in the unperturbed basis naturally depend on \( \alpha \). However, when it is evaluated on-energy-shell as expressed by the delta-function in the S-matrix element \( S_{nm} \), all \( \alpha \)-dependence drops out [35, 74]. This bare-energy conservation property is thereby seen to be crucial in ensuring that the gauge-relativity of the subsystems can be ignored when calculating the S-matrix.

We can define any process that conserves \( h \) as real. A virtual process is then one that is not real. In the S-matrix, the latter can only occur as intermediate processes constituting part of a real process. More generally, however, the S-matrix can be understood as an infinite-time limit of the more general matrix given by [75]

\[
S^{(\tau)}_{nm} = \delta_{nm} - 2\pi i T_{nm}\delta^{(\tau)}(\epsilon_n - \epsilon_m)
\]

(181)

The function \( \delta^{(\tau)}(\epsilon_n - \epsilon_m) \) has a peak at \( \epsilon_n = \epsilon_m \) with width on the order \( 1/\tau \), which is often taken as expressing the conservation of bare energy to within \( 1/\tau \) [75]. This is the heuristic energy-time uncertainty relation, which it should be noted is quite different to the rigorous Heisenberg uncertainty relation for conjugate operators. However, it is clear that the processes described by the matrix \( S^{(\tau)} \) are not purely real (zero energy-uncertainty) unless \( \tau \to \infty \).

It is widely regarded that physical processes are “real”. However, although the total energy \( E \) represented by the operator \( H_\alpha \) is automatically conserved, there is nothing in quantum or classical theory that requires a physical process to conserve only part of this energy, such as the part represented by \( h \). This is required and does occur in the S-matrix only because \( H_\alpha = h \) at the beginning.
and the end of a scattering process. And yet, the limit of infinite times with adiabatic switching is clearly an idealisation, such that purely “real” processes cannot truly occur. In this sense the term “real” is a misnomer. Further still, it is clear that only when a process is “real”, i.e., is a scattering process, can the gauge-relativity of the subsystems necessarily be ignored.

All predictions are fundamentally gauge-invariant in the sense of Eq. (177). Thus, both sides of inequality (178) are gauge-invariant predictions, but beyond scattering theory, i.e., over finite-times, we must recognise that they are different gauge-invariant predictions. Each different $\alpha$ corresponds to a different physical definition of the subsystems. Outside of scattering theory we must confront the question as to which of the many gauge-invariant subsystem definitions are relevant in which physical situations. For example, in a physical situation where we are unable to use the $S$-matrix, Eq. (180), then which side of inequality (178) provides the most relevant prediction?

As an analogy consider special relativity; suppose we were to adopt the definition of time that is provided by a specific inertial frame $A$ to predict the outcome of a measurement from a clock that is at rest in frame $B$. In general, this would result in an incorrect prediction, because we would have used a definition of time that although a valid physical definition, is not relevant in describing the measurement being performed. Only within the nonrelativistic regime can intervals in time be considered frame-independent (absolute as opposed to relative). Similarly, scattering theory constitutes a completely gauge-nonrelativistic theory. In any other situation, for example, when interactions are fast and strong, the gauge-relativity of subsystems is important, such that we are no longer able to pretend that quantum subsystems are absolute (gauge-frame independent). We must then identify which definitions are relevant in which physical situations.

### B. Quantum optical approximations: Mimicking the $S$-matrix

We directly demonstrate that subsystem gauge-relativity is eliminated only after a sufficient number of weak-coupling approximations are performed, in which case “light” and “matter” as quantum subsystems, become ostensibly unique theoretical concepts.

1. **Toy model: material oscillator and a single mode**

We begin by using a simple toy model that as above assumes a material harmonic oscillator. We now also consider only a single radiation mode, such that Eqs. (14) and (9) become

$$P_{T\alpha} = \frac{\alpha q x}{v}, \quad (182)$$

$$A_\alpha = (1 - \alpha)A \quad (183)$$

where $v$ is the cavity volume. The cavity canonical operators are

$$A = \frac{1}{\sqrt{2\omega v}}(a^\dagger + a), \quad (184)$$

$$\Pi = i\sqrt{\frac{\omega}{2v}}(a^\dagger - a) \quad (185)$$

such that $[A, \Pi] = i/v$. We assume that the material oscillator points in the same direction as the mode. The theory is gauge-invariant because gauge-fixing transformations remain unitary; $R_{\alpha\alpha'} = e^{i\beta(\alpha - \alpha')rA}$.

The $\alpha$-gauge Hamiltonian in Eq. (22) can be written $H^\alpha = h + V^\alpha$ where $h = \omega(a^\dagger a + 1/2) + \omega_m(b^\dagger b + 1/2)$ and

$$V^\alpha = \frac{\eta^2}{4} \omega \left[ (1 - \alpha)^2(a^\dagger a + b^\dagger b)^2 +\right.\
+ i\eta\alpha(\alpha^\dagger a + b^\dagger b) + i\eta^2\alpha^\dagger \alpha b^\dagger a - \left. \alpha b\right] \quad (186)$$

with $\eta = -q/(\omega \sqrt{m})$ a dimensionless coupling parameter, $\delta = \omega/\omega_m$, and

$$u^\pm_\alpha = \frac{\eta\omega_m}{2} \sqrt{\delta}(1 - \alpha) \pm \delta \alpha \tag{187}$$

Clearly the value of $\alpha$, which determines the physical definitions of the two oscillator subsystems, can have a profound affect on the form of $V^\alpha$. This is completely eliminated however, if we assume weakly-coupled nearly-resonant oscillators. We can then let $\omega_m = \omega$, and we can neglect terms quadratic in $\eta$. We can also perform the rotating-wave approximation by setting $u^\pm_\alpha = 0$. The final result is the $\alpha$-independent Hamiltonian $H = h + V$ where $h = \omega(a^\dagger a + b^\dagger b + 1)$ and

$$V^\alpha = V = \frac{i}{2} \omega \eta(ab^\dagger - a^\dagger b). \quad (188)$$

This Hamiltonian satisfies bare-energy conservation

$$[h, H] = 0, \tag{189}$$

which we saw in the context of the $S$-matrix was crucial in eliminating subsystem gauge-relativity. We have obtained the same result here in a very direct manner. We can now pretend that the two oscillators represent unique physical subsystems.

Outside of the regime of validity of weak-coupling approximations, it is typically thought that one cannot let $u^\pm_\alpha \approx 0$. In general, this is true, by which we mean that one can only use this approximation independent of the value of $\alpha$ in the weak-coupling regime. However, whether $V^\alpha$ includes counter-rotating terms depends on the value of $\alpha$, so there exists a range of values...
for which the rotating-wave approximation will remain valid well into the ultrastrong coupling regime. For a specific choice of $\alpha$ the rotating-wave approximation is exact \cite{4, 5, 14, 15, 71}. Specifically, by choosing $u_+ = 0$, so the counter-rotating terms in the bilinear component of $V^\alpha$ in Eq. (186) are automatically eliminated. As before, by performing non-mixing Bogoliubov transformations within the separate light$_{\text{JC}}$ and matter$_{\text{JC}}$ Hilbert spaces, we can eliminate terms quadratic in $\eta$ via modes $c$ and $d$ such that

$$\alpha(\omega) = \alpha_{\text{JC}}(\omega) := \frac{\omega_m}{\omega_m + \omega}$$

we obtain $u^+_+ \equiv 0$, so the counter-rotating terms in the bilinear component of $V^\alpha$ in Eq. (186) are automatically eliminated. As before, by performing non-mixing Bogoliubov transformations within the separate light$_{\text{JC}}$ and matter$_{\text{JC}}$ Hilbert spaces, we can eliminate terms quadratic in $\eta$ via modes $c$ and $d$ such that

$$\frac{p^2}{2m} + \frac{m\omega_m^2}{2} + \frac{q^2}{2v} \alpha_{\text{JC}}^2 r^2 = \tilde{\omega}_m \left( d^d + \frac{1}{2} \right),$$

$$\frac{v}{2} (\Pi^2 + \omega^2 A^2) + \frac{q^2}{2m} (1 - \alpha_{\text{JC}})^2 A^2 = \tilde{\omega} \left( c^\dagger c + \frac{1}{2} \right)$$

where

$$\tilde{\omega}_m^2 = \omega_m^2 + \omega^2 \eta^2 \alpha_{\text{JC}}^2 = \omega_m^2 \mu,$$

$$\tilde{\omega}^2 = \omega^2 + \omega^2 \eta^2 (1 - \alpha_{\text{JC}})^2 = \omega^2 \mu$$

in which

$$\mu = 1 + \left( \frac{\eta \omega_d}{\omega_m + \omega} \right)^2.$$  

In the single-mode case this elimination of self-energy terms is exact. It follows that $\alpha_{\text{JC}}$ can be written $\alpha_{\text{JC}} = \tilde{\omega}_m / (\tilde{\omega} + \tilde{\omega}_m)$. The corresponding Hamiltonian is

$$H_{\text{JC}} = \tilde{\omega}_m \left( d^d + \frac{1}{2} \right) + \tilde{\omega} \left( c^\dagger c + \frac{1}{2} \right)$$

$$- i q \sqrt{\frac{\omega_m}{m} \left( \frac{1}{2} \omega_m \right)} \frac{1}{\omega_m + \omega} (d^d c - d c^\dagger),$$

The ground state is represented by the the vacuum of the $c$ and $d$ modes; $|G_{\text{JC}}\rangle = |0_d, 0_c\rangle$. We emphasise that at no point have we made use of any approximations or assumptions that ruin the gauge-invariance of the theory. Neither however, have we performed a diagonalising transformation of the Hamiltonian. We have simply considered a particular definition of the subsystems specified by a value $\alpha_{\text{JC}}$ in between the commonly chosen values $\alpha = 0$ and $\alpha = 1$, and within this gauge we have only performed non-mixing Bogoliubov transformations of the form $U_m \otimes U_{\text{ph}}$. Whether or not the latter transformations are employed counter-rotating terms are absent, because $u^+_+ \equiv 0$. Thus,

- It is premature to define the paradigm of extreme-coupling light-matter physics through properties such as high-levels of ground-state light-matter entanglement and photon population, which only result from terms that happen to feature in commonly chosen gauges, but which are not necessarily present.

There are no ground state virtual excitations in the modes $c$ and $d$ when they are defined relative to the gauge $\alpha_{\text{JC}}$. We will see in Secs. VB and VC2 that as a result, “matter” cannot be fully localised in this gauge. Finally we remark that although a projection $P = |0_d\rangle \langle 0_d| + |1_d\rangle \langle 1_d|$ onto the first two levels of the material oscillator is as ill-justified as it can ever be (because the material system has zero anharmonicity), such a projection nevertheless yields the exact ground state; $P |G_{\text{JC}}\rangle = |G_{\text{JC}}\rangle$. This fact is relevant to our discussion of material truncation in Sec. III.

2. Quantum optical master equation

We now turn our attention to a more realistic setting by deriving the quantum optical master equation for the dipole$_{\alpha}$, which can be viewed as a detector for the corresponding $\alpha$-gauge radiation field. In general, such a reduced description will of course depend on $\alpha$. However, we will show that the weak-coupling approximations comprising the traditional quantum optics paradigm, have the effect of mimicking the $S$-matrix and they thereby cause all $\alpha$-dependence to drop out of the final result. More precisely, they ensure that all master equation coefficients are well-known second-order QED matrix elements. A similar demonstration has been given for a pair of two-level dipoles in Ref. \cite{71}. Here we consider only one dipole (the detector), but we do not restrict our attention to only two dipolar energy levels.

We make the following weak-coupling approximations concerning the state of the detector$_{\alpha}$ represented by the density operator $\rho(t)$ in a suitably chosen interaction picture:

1. Born approximation: The dipole and reservoir are uncorrelated over the relevant timescale.
2. Second order perturbation theory: The coupling is much smaller than the unperturbed energies.
3. Markov approximation A: The system dynamics are memoryless; $\rho(s) \approx \rho(t)$ for all $s \in [0, t]$.
4. Markov approximation B: The temporal limit of the integrated Von-Neumann equation is $t \approx \infty$.
5. Secular (rotating-wave) approximation: Rapidly oscillating contributions are negligible.

The Markov approximations mimic the adiabatic switching condition of the $S$-matrix and together with the secular approximation they enforce bare-energy conservation. The steps involved in deriving the quantum optical master equation are well-known \cite{76}, but we will repeat them here using an arbitrary gauge in order to show how approximations 1-5 cause all $\alpha$-dependence to drop out of the final result. We use the EDA of the arbitrary gauge
Hamiltonian in Eq. (22), which is
\[ H = h + V_1^\alpha + V_2^\alpha \] (197)
\[ h = \sum_n e^n |e^n\rangle \langle e^n| + \int d^3k \sum_{\lambda} \omega \left( a_\lambda^\dagger(k)a_\lambda(k) + \frac{1}{2} \right), \] (198)
\[ V_1^\alpha = -(1 - \alpha) \frac{q}{2m} \mathbf{p} \cdot \mathbf{A}_T(0) + \alpha \eta \mathbf{q} \cdot \mathbf{r} \] (199)
\[ V_2^\alpha = (1 - \alpha)^2 \frac{q^2}{2m} \mathbf{A}(0)^2 + \alpha \frac{q^2}{2} \mathbf{r} \cdot \mathbf{r} \cdot \mathbf{T}(0) \cdot \mathbf{r}. \] (200)
The terms \( h, V_1^\alpha, \) and \( V_2^\alpha \) are zeroth, first, and second order in \( q \) respectively \((q^2/(4\pi)\) is the fine structure constant serving as a dimensionless small parameter). Despite the EDA, the theory remains gauge-invariant because \( R_\alpha \) remains unitary.

We will view \( h \) as the unperturbed Hamiltonian, whose definition we have made sure to keep independent of \( \alpha \), because this is essential in order that the \( S \)-matrix is \( \alpha \)-independent (cf. Sec IV A). In approximation 1 we assume that the system’s density matrix can be written \( \rho(t) \otimes |0\rangle \langle 0| \) where \(|0\rangle \) is the photonic vacuum and \( \rho(t) \) is the dipole state in the interaction picture with respect to \( h \). In approximation 2 the Von-Neumann equation for the density matrix is integrated and iterated up to second order in \( q \) to give [76]
\[ \dot{\rho}(t) = i[\rho(0), \Delta_2^\alpha(t)] \]
\[ - \int_0^t ds \mathrm{tr}_{\mathrm{ph}} [V_1^\alpha(t), [V_1^\alpha(t - s), \rho(s) \otimes |0\rangle \langle 0|]] \] (201)
where \( \Delta_2^\alpha(t) := |0\rangle \langle 0| V_2^\alpha(t) |0\rangle \). In approximation 3 the density matrix \( \rho(s) \) is approximated as \( \rho(s) \approx \rho(t) \) for all \( s \in [0, t] \) resulting in the time-local equation
\[ \dot{\rho}(t) = i[\rho(t), \Delta_2^\alpha(t)] \]
\[ - \int_0^t ds \mathrm{tr}_{\mathrm{ph}} [V_1^\alpha(t), [V_1^\alpha(t - s), \rho(t) \otimes |0\rangle \langle 0|]] . \] (202)

In principle, all terms can now be calculated as known functions of \( t \) that are second order in \( q \). In approximation 4 the limit of integration is extended; \( t \to \infty \), which gives the Markovian equation
\[ \dot{\rho}(t) = \]
\[ i[\rho(t), \Delta_2^\alpha(t)] - \int_0^\infty ds \langle 0| V_1^\alpha(t)V_1^\alpha(t - s) |0\rangle \rho(t) \]
\[ - \mathrm{tr}_{\mathrm{ph}} [V_1^\alpha(t) |0\rangle \langle 0| V_1^\alpha(t - s)] + \text{H.c.} \] (203)
Typically the \( s \)-integral will not converge and must be appropriately regularised. In the Schrödinger-picture, all master equation coefficients will now be time-independent. Having used approximations 1–4 the complete positivity of the reduced evolution is not guaranteed. Complete positivity requires approximation 5 [76].

We will first deal with the unitary part of the master equation, which is given by
\[ \dot{\rho}(t)|_{u} = i[\rho(t), \Delta^\alpha(t)] \] (204)
where \( \Delta^\alpha(t) = \Delta_2^\alpha(t) + \Delta_3^\alpha(t) \) in which \( \Delta_3^\alpha(t) \) comes from partitioning the coefficient of \( \rho(t) \) in the second term in Eq. (203) as
\[ \int_0^\infty ds \langle 0| V_1^\alpha(t)V_1^\alpha(t - s) |0\rangle = \gamma^\alpha(t) + i\Delta_3^\alpha(t). \] (205)
The dipole operators \( \gamma^\alpha(t) \) and \( \Delta_3^\alpha(t) \) will be seen in the end to be separately Hermitian. We will now show that within approximation 5 we obtain
\[ \Delta^\alpha(t) = \sum_n \Delta_n |e^n\rangle \langle e^n| \] (206)
where \( \Delta_n \) is the \( \alpha \)-independent on-energy-shell second order \( T \)-matrix element for the vacuum shift of the dipole’s \( n \)’th energy level;
\[ \Delta_n = \langle e^n, 0| V_2^\alpha |e^n, 0 \rangle + \sum_{m \neq n} \frac{|\langle e^n| V_1^\alpha |e^m, 0 \rangle|^2}{\epsilon_n - \epsilon_m} . \] (207)
Here the summation is over all unperturbed states \(|e^m\rangle \neq |e^n\rangle \). Direct calculation yields
\[ \int_0^\infty ds \langle 0| V_1^\alpha(t)V_1^\alpha(t - s) |0\rangle = \int d^3k \sum_{n,m,q} \]
\[ \times g_{nm\lambda} g_{mq\lambda} u_{nm\alpha}^+ v_{mq\alpha}^- \langle e^q \rangle \langle \epsilon | e^{\omega_{nq}t} \int_0^\infty ds e^{i(\omega_{q} - \epsilon)s} \] (208)
where \( \omega_{nm} := \epsilon_n - \epsilon_m \) and
\[ g_{nm\lambda} := \frac{q e_\lambda(k) \cdot r_{nm}}{\sqrt{2\omega(2\pi)^3}} , \] (209)
\[ u_{nm\alpha}^+ := \alpha \omega \pm (1 - \alpha) \omega_{nm} . \] (210)
Forcing the \( s \)-integral in Eq. (208) to converge by adding damping \( e^{-\eta s} \), \( \eta \to 0_+ \), and using the identity
\[ \lim_{\eta \to 0_+} \int_0^\infty ds e^{i\delta_\eta s} e^{-\eta s} = \pi \delta(\epsilon) + i \frac{\mathrm{D.V.}}{\epsilon} \] (211)
the quantity \( \Delta_1^\alpha(t) \) is identified as the component of Eq. (208) coming from the principal value term;
\[ \Delta_1^\alpha(t) \]
\[ = \int d^3k \sum_{\lambda} \sum_{n,m,q} g_{nm\lambda} g_{mq\lambda} \frac{u_{nm\alpha}^+ v_{mq\alpha}^-}{\omega_{qm} - \epsilon} \langle e^q \rangle \langle \epsilon | e^{\omega_{nq}t} \] (212)
where the \( k \)-integral takes its principal value. For the term \( \Delta_2^\alpha(t) \) direct calculation yields
\[ \Delta_2^\alpha(t) = \int d^3k \sum_{\lambda} \left( \frac{(1 - \alpha)^2 q^2 |e_\lambda(k)|^2}{4m\omega(2\pi)^3} + \sum_{n,m,q} \alpha^2 \omega g_{nm\lambda} g_{mq\lambda} \langle e^n \rangle \langle \epsilon | e^{\omega_{nq}t} \right) \] (213)
and using the Thomas-Reich-Kuhn identity
\[
\frac{1}{2m} \delta_{ij} = \sum_n \omega_{mn} r_{nm,i} r_{mn,j}
\] (214)
we obtain
\[
\Delta_2^\alpha(t) = \int d^3 k \sum_{\lambda,n,m} \left( (1 - \alpha)^2 \omega_{mn} |g_{nm\lambda}|^2 \langle \epsilon^n \rangle \langle \epsilon^n \rangle + \sum_q \alpha^2 \omega_{mn\lambda} g_{mq\lambda} |\epsilon^n \rangle \langle \epsilon^q | e^{i\omega_{nq} t} \right).
\] (215)

In approximation 5 the off-diagonal terms in \(\Delta_2^\alpha(t)\) and \(\Delta_3^\alpha(t)\) for which \(q \neq n\) are assumed to be rapidly oscillating and are ignored. We thereby obtain
\[
\Delta_2^\alpha = \int d^3 k \sum_{\lambda,n,m} |g_{nm\lambda}|^2 \left[ (1 - \alpha)^2 \omega_{mn} + \alpha^2 \omega \right] \langle \epsilon^n \rangle \langle \epsilon^n \rangle
\] (216)
\[
\Delta_3^\alpha = \int d^3 k \sum_{\lambda,n,m} |g_{nm\lambda}|^2 \left[ (1 - \alpha) \omega_{nm} + \alpha \omega \right] \langle \epsilon^n \rangle \langle \epsilon^n \rangle.
\] (217)

These terms give respectively the contributions of \(V_2^\alpha\) and \(V_3^\alpha\) to the right-hand side of Eq. (207). Their sum is therefore \(\alpha\)-independent and is found to be
\[
\Delta^\alpha = \Delta = \sum_n \Delta_n \langle \epsilon^n \rangle \langle \epsilon^n \rangle
\] (218)

Let us recap how this result has been obtained. Approximation 1 ensured that \(\Delta^\alpha(t)\) could be calculated using the photonic vacuum at any time \(t\). Approximation 2 ensured that it was of second order in \(q\). Approximation 3 ensured it could be calculated independent of \(\rho\). Approximation 4 ensured that the expected energy denominators were obtained as in the \(T\)-matrix, and approximation 5 ensured that the \(T\)-matrix element was evaluated on-energy-shell. It follows that the unitary part of the master equation [Eq. (204)] is \(\alpha\)-independent.

We now consider the dissipative part. We first calculate \(\gamma^n(t)\) defined by Eq. (205), which is the remaining component of Eq. (208) that comes from the delta-function term of Eq. (211);
\[
\gamma^n(t) = \int d^3 k \sum_{\lambda,n,m,q} \pi g_{nm\lambda} g_{mq\lambda} u_{nm} u_{mq} e^{i\omega_{nq} t} \delta(\omega_{qm} - \omega) |\epsilon^n \rangle \langle \epsilon^q |.
\] (219)

We see immediately that approximation 4 has resulted in an evaluation of the photonic frequencies on resonance with dipolar transitions. Invoking the approximation 5 of neglecting terms for which \(q \neq n\) we obtain
\[
\gamma^n(t) = \gamma = \int d^3 k \sum_{\lambda,n,m} \pi |g_{nm\lambda}|^2 (1 - \alpha) \omega_{nm} + \alpha \omega \delta(\omega_{nm} - \omega) |\epsilon^n \rangle \langle \epsilon^n |
\] (220)
\[
= \sum_{n,m} \int d^3 k \lambda \pi |g_{nm\lambda}|^2 \alpha^2 \omega_{nm} \delta(\omega_{nm} - \omega) |\epsilon^n \rangle \langle \epsilon^n |.
\]

where in the final equality all \(\alpha\)-dependence has dropped out due to the delta function. Within the approximations 1-5 the coefficient in the summand over dipole levels is half the rate of emission into the photonic continuum via a downward transition \(|\epsilon^n \rangle \rightarrow |\epsilon^m \rangle\), the latter being exactly as is found using the corresponding \(S\)-matrix element. This calculation is also commonly called Fermi’s golden rule [53]. Evaluating the \(k\)-integral and polarisation summation we obtain
\[
\gamma = \sum_{n,m} \frac{\Gamma_{nm}}{2} |\epsilon^n \rangle \langle \epsilon^n |.
\] (221)
\[
\Gamma_{nm} = \frac{q^2 \omega_{nm} |g_{nm\lambda}|^2}{3\pi}.
\]

The remaining part of the master equation is another dissipative part coming from the second line in Eq. (203). This can be calculated in a similar fashion using Eq. (211) and approximation 5. The final coefficients are again found to be the \(\alpha\)-independent \(\Gamma_{nm}\). Collecting these results we obtain the quantum optical master equation at zero temperature [76], which in the Schrödinger picture reads
\[
\dot{\rho} = i[\rho, \hat{H}_d] + \sum_{n,m} \Gamma_{nm} \left( L_{nm}\rho L_{nm}^\dagger - \frac{1}{2} \{ L_{nm}^\dagger L_{nm}, \rho \} \right)
\] (222)

where \(\hat{H}_d = \hat{H}_d + \Delta\) and the Lindblad operators are simply \(L_{nm} = |\epsilon^m \rangle \langle \epsilon^n |.\) The result is readily extended to finite temperature [76]. Clearly:

- The reduced description of the detector \(\alpha\) is \(\alpha\)-independent within the approximations 1-5, such that “detector” becomes an ostensibly unique theoretical concept.

The stationary state \(\rho_0\) of this detector is the bare ground state
\[
\rho_0 = |\epsilon^0 \rangle \langle \epsilon^0 |,
\] (223)
according to which the probability of excitation of the detector initially in the ground state is \(\mathcal{P}_d(0) = 0\) for all \(t\). Within the approximations made photon emission requires a downward dipolar transition and absorption an upward one. Furthermore, the energies of any photons involved must be exactly equal to the energies of the corresponding dipolar transitions involved. The processes
captured by the master equation (222) are precisely those captured by the $S$-matrix wherein $\hbar$ is strictly conserved.

Outside of the approximations 1-5 emission and absorption can occur without preserving the number of bare quanta, but evidently such (“virtual”) processes are not perfectly bare-energy conserving and they are non-secular and/or non-Markovian inasmuch that they are only eliminated when both Markov and secular approximations are performed. These processes are allowed (not only as intermediates) by the more general matrix $S(t)$ defined in Eq. (181) and although they are viewed as unphysical in scattering theory (except as intermediates), in open quantum systems theory the opposite is true; they are allowed unless they have been suppressed by approximations whose avoidance must provide a more accurate description. Moreover, these approximations have a relatively narrow regime of validity [76]. There is presently considerable interest within open quantum systems theory in understanding strong-coupling and non-Markovian effects using both numerical and analytical methods [77–81]. From this perspective, when the approximations 1-5 breakdown the idealisations used to define the $S$-matrix must be interpreted as no longer realistic.

C. Time-dependent interactions and ground state photons

We now turn our attention to non-adiabatic interaction switching whereby the gauge-relativity of subsystems cannot be ignored. It is sometimes argued that the Coulomb gauge must be used to describe residual photon population left after a sufficiently fast interaction switch-off (e.g. Ref. [7, 10]). In fact, the correct description depends on the experimental context [5] as will be discussed in detail below. Recently, Refs. [5, 10] have considered time-dependent interactions with non-adiabatic switching in the context of ground state photon production.

The ground state of a light-matter system is gauge-invariant, but its representation using a vector differs between gauges (see Sec. II K). This gives rise to different photon number predictions all of which are physical. The different predictions within one and the same physical state correspond to different gauge-invariant definitions of a photon. The task remains of determining which gauge-invariant prediction is most relevant in any given situation? Towards providing an answer, let us consider a system prepared in the ground state before we suddenly switch-off the interaction. When the interaction is suddenly switched-off at $t > t_f$? Modelling this situation using a time-dependent coupling in the gauge $\alpha$ gives the Hamiltonian

$$H_\alpha(t) = H_m + H_{ph} + \theta(t - t_f) V^\alpha(\eta)$$

where the vector $|G_{\alpha}\rangle = |E_{\alpha}\rangle$ represents the ground state in the gauge $\alpha$ and where $a_{\lambda}(k)$ is defined in Eq. (99). At first glance it seems that the predicted photon number $N_\alpha$ is fundamentally gauge-noninvariant, and that this is because $|G_{\alpha}\rangle$ depends on $\alpha$, but this is not the case. Rather, the operator $n$ represents the gauge-invariant number of photons defined relative to the gauge $\alpha$. In the gauge $\alpha'$ the same observable is represented by $n' = R_{\alpha\alpha'} n R_{\alpha\alpha'}^\dagger$ and the physical ground state is represented by the vector $|G_{\alpha'}\rangle = R_{\alpha\alpha'} |G_{\alpha}\rangle$. Thus, $N_\alpha$ is gauge-invariant;

$$N_\alpha = \langle G_{\alpha}|n|G_{\alpha}\rangle = \langle G_{\alpha}|n'|G_{\alpha'}\rangle.$$  

(225)

For each different fixed value of $\alpha$ the average $N_\alpha$ is that of a different physical observable and it is therefore a different gauge-invariant prediction. The subscript $\alpha$ labels which particular gauge-invariant definition of photon is being considered. A special case is the number of $E_T$-type photons given by $N_0 =: |N_{E_T}|$ because $\Pi(k) = -E_T(k)$ when $\alpha = 0$. Another special case is the number of $D_T$-type photons, which is given by $N_1 =: |N_{D_T}|$, because $\Pi(k) = -D_T(k)$ when $\alpha = 1$.

An obvious question to ask is; which gauge-invariant prediction $N_\alpha$ is most relevant in any given situation? Towards providing an answer, let us consider a system prepared in the ground state before we suddenly switch-off the interaction. When the interaction is suddenly switched-off at $t > t_f$ if the interaction is suddenly switched-off at $t = t_f$? Modelling this situation using a time-dependent coupling in the gauge $\alpha$ gives the Hamiltonian

$$H_\alpha(t) = H_m + H_{ph} + \theta(t - t_f) V^\alpha(\eta)$$

where $\theta$ is the heaviside step-function and $\eta$ is a coupling parameter such that $V^\alpha(0) = 0$. These $H_\alpha(t)$ are clearly not equivalent to each other for different $\alpha$ [5]. This is unsurprising because for $\alpha \neq \alpha'$, $H_\alpha(t)$ and $H_{\alpha'}(t)$ clearly model two different experiments in which $V^\alpha$ and $V^{\alpha'}$ are suddenly switched-off, respectively. For each $\alpha$ the evolution generated by $H_\alpha(t)$ from time $t = 0$ consists of sequential evolutions; $U_\alpha(t) = e^{-i(H_m + H_{ph})(t - t_f)} e^{-iH_\alpha t_f}$. It follows that the gauge-invariant physical prediction $N_\alpha =: |N_{E_T + \alpha P_T}|$ gives by Eq. (225) gives the number of photons left over in an experiment that realises a sudden switch-off of the $\alpha$-gauge interaction.

Every prediction is gauge-invariant, but gauge-ambiguities arise because it is not immediately obvious
which prediction is relevant for describing a given real-world setup. Does a given setup realise a sudden switch-off of the Coulomb-gauge interaction or the multipolar-gauge interaction, or does it realise neither? In the recent article [10], for example, it is noted that the particular prediction $N_0 = N_{E^0}$ is gauge-invariant, but as we have shown more generally the same is true of any of the predictions $N_\alpha$. Ref. [10] considers a single-mode resonator and states that $N_0$ can be observed as the output photon flux from the resonator after a sudden switch-off of the interaction. If this were found to be the case experimentally, it would simply follow that the particular protocol adopted can be modelled as a sudden switch-off of the Coulomb-gauge interaction.

However, there is a famous set of experiments for which it is well-known that the sudden switching condition is ill-justified in the Coulomb-gauge as compared with the multipolar-gauge, these being the early experiments of Lamb [33–36, 82]. The natural lineshape prediction can be obtained by assuming the atom to be initially in a bare excited state with no photons. This amounts to a sudden switch-on of the interaction [34]. Within the multipolar gauge the prediction is sufficiently close to the experimental result to rule out the corresponding Coulomb-gauge prediction [33–36]. Put differently, the multipolar-gauge subsystems are more operationally relevant when describing this experiment.

It should be clear that one can consider more general time-dependent interactions and the same considerations will apply. The generalisation can be achieved by letting

$$H_\alpha(t) = H_m + H_{ph} + V^\alpha(\eta\mu(t))$$

(227)

where $\mu(t)$ is an arbitrary coupling envelope that vanishes smoothly after some time $t_f$. Let us also suppose, as in Ref. [5], that $\mu(t)$ vanishes before some time $t_i$ so the system can be prepared in a bare state. Suppose the system is prepared at $t = 0 < t_i$ in the ground state represented by the vector $|g\rangle = |e^0\rangle$ such that $h|g\rangle = e^0|g\rangle$, then the total number of photons at time $t > t_f$ is

$$N_\alpha(t) = \langle g| U_\alpha(t) n U_\alpha(t)\dot{t} |g\rangle$$

(228)

where $U_\alpha(t)$ is the evolution operator generated by $H_\alpha(t)$. To prove the gauge-invariance of $N_\alpha(t)$ one must of course take into account that gauge transformations are now time-dependent, because they depend on the coupling parameter; $R_{\alpha\alpha'}(\eta\mu(t)) \equiv R_{\alpha\alpha'}(t)$. The vector $|g_\alpha(t)\rangle = U_\alpha(t)|g\rangle$ represents the Schrödinger-picture state at time $t$ in the gauge $\alpha$. The same physical state is represented in the gauge $\alpha'$ by the vector $|g^\alpha_\alpha(t)\rangle = R_{\alpha\alpha'}(t)|g_\alpha(t)\rangle$. The physical observable represented by $n$ in the Schrödinger picture in the gauge $\alpha$ is represented by $n^\alpha(t) = R_{\alpha\alpha'}(t) n R_{\alpha\alpha'}(t)\dot{t}$ in the gauge $\alpha'$. We see immediately therefore, that $N_\alpha(t)$ is a gauge-invariant prediction.

The two different vector representations $|g_\alpha(t)\rangle$ and $|g^\alpha_\alpha(t)\rangle$ of the state at $t$, satisfy the respective Schrödinger equations

$$i\frac{d}{dt}|g_\alpha(t)\rangle = H_\alpha(t)|g_\alpha(t)\rangle,$$  \hspace{2cm} (229) 

$$i\frac{d}{dt}|g^\alpha_\alpha(t)\rangle = H_{\alpha'}^\alpha(t)|g^\alpha_\alpha(t)\rangle.$$  \hspace{2cm} (230)

The Hamiltonians $H_{\alpha'}^\alpha(t)$ and $H_\alpha(t)$ are easily related via direct differentiation of the expression $|g^\alpha_\alpha(t)\rangle = R_{\alpha\alpha'}(t)|g_\alpha(t)\rangle$, which implies

$$H_{\alpha'}^\alpha(t) = R_{\alpha\alpha'}(t) H_\alpha(t) R_{\alpha\alpha'}(t)\dot{t} + \dot{R}_{\alpha\alpha'}(t) R_{\alpha\alpha'}(t)\dot{t}.$$  \hspace{2cm} (231)

Thus, we see that it is a trivial matter to generate an equivalent model to any one of the $H_\alpha(t)$ by properly accounting for the time-dependence of gauge transformations. For fixed $\alpha$ the equivalent Hamiltonians $\{H_{\alpha'}^\alpha(t)\}$ can also be derived from equivalent Lagrangians, any two of which differ by a total time-derivative.

The Hamiltonian $H_{\alpha'}^\alpha(t)$ depends on two parameters $\alpha$ and $\alpha'$ which have different roles. The parameter $\alpha$ selects the gauge within which the time-dependent coupling assumption has been made whereas the parameter $\alpha'$ selects the choice of gauge used for calculations once this assumption has been made. The equivalence of the $H_{\alpha'}^\alpha(t)$ for different $\alpha'$ shows that following the physical assumption $e \rightarrow e(t)$ made in gauge $\alpha$, the description by $H_\alpha(t)$ is gauge-invariant. The non-equivalence of the $H_\alpha(t)$ for different $\alpha$ shows that the assumption $e \rightarrow e(t)$ constitutes a different physical assumption in different gauges. In other words, gauge-ambiguities arise because each $H_\alpha(t)$ generates its own equivalence class as

$$S_\alpha = \{H_{\alpha'}^\alpha(t) : \alpha' \in \mathbb{R}\}$$

(232)

and distinct classes describe different experiments. The particular prediction $N_\alpha(t)$ is relevant if the experimental protocol being modelled happens to realise a switch-on/off of the interaction $V_\alpha$. If, for example, the experimental arrangement considered is somehow capable of effectively manipulating the (gauge-invariant) bare dipole moment $q\vec{r}$, then the multipolar-gauge interaction could be controlled to some extent.

These points are demonstrated directly in Ref. [5], which considers the concrete setup of a dipole uniformly moving in and out of a Gaussian cavity mode, as depicted in Fig. 6. This situation can be modelled using a Gaussian envelope $\mu(t)$. In addition to the non-equivalent models $H_\alpha(t)$, a more complete description $H_\alpha(t)$ is provided by retaining an explicit model for the control system, which in this example is the centre-of-mass motion of the dipole. Unlike the $H_\alpha(t)$ the more complete descriptions $H_\alpha(t)$ are equivalent to each other for different $\alpha$. The value of $\alpha$ such that $H_\alpha(t) = H_\alpha(t)$ is then the correct value to choose when describing the experiment using the simpler model $H_\alpha(t)$. Thus, the procedure of using a time-dependent coupling $\eta(t)$ can be viewed as an approximation of a more complete description. The
FIG. 6: A cavity of length $L$ demonstrating that in general, which prediction $N_w$ with waist $z$ the non-interacting. The dipole follows a classical trajectory $R(t)$ through the cavity, entering the cavity at $t_0$ and exiting at $t_0 + \tau$.

value of $\alpha$ for which $\tilde{H}_\alpha(t) = H_\alpha(t)$ gives the corresponding prediction $N_\alpha(t)$ that must correctly give the number of photons left in the cavity at the end of the protocol, i.e., after the interaction has ceased (the dipole has fully passed through the cavity).

It is shown in Ref. [5] that if there exists a value $\alpha$ for which $\tilde{H}_\alpha(t) = H_\alpha(t)$, then the value depends strongly on the experimental protocol. In other words, which prediction $N_\alpha(t)$ (if any) correctly predicts the number of photons left in the cavity after the atom has passed through, depends strongly on the experimental context. The prediction $N_\alpha(t)$ is correct if and only if the dipole moment is aligned with the mode polarisation and these vectors make an angle $\theta$ with the direction of the centre-of-mass motion, such that $\cos^2 \theta = \alpha$. The result clearly demonstrates that in general, which prediction $N_\alpha(t)$ is the correct (relevant) one, depends strongly on the experimental context. It is certainly not the case that $N_0(t)$ is always the correct prediction. The result further illustrates why there are indeed gauge-ambiguities. In order to find which of the predictions $N_\alpha(t)$ may be relevant for describing a concrete setup and experimental protocol, Ref. [5] resorts to invoking an explicit model of the control system. The result obtained could not be anticipated without such a description, and yet such descriptions are only available in the simplest of cases whereby the control system accommodates tractable modelling.

V. MEASUREMENTS

We now turn to the topic of subsystem measurements. We focus on a system consisting of a source and/or a detector within a single photonic environment which is either free space or a photonic cavity. This situation is distinguished from the case of a source and a detector occupying different environments that are modelled separately, such as a source within a cavity with a detector external to the cavity. The outlook for this latter situation is only briefly discussed at the end in Sec. VD4.

The natural starting point for our considerations is Glauber’s photodetection theory [60, 83]. We review aspects of photodetection that are important beyond the standard quantum optics paradigm including how photodetection divergences are related to virtual excitations. We determine the relation between subsystem gauge-relativity and locality, and how virtual ground state excitations are related to various electromagnetic energy densities in the vicinity of a detector.

The important conclusion of this section is that outside of conventional weak-coupling and Markovian regimes there is necessarily a trade-off between defining material systems as localised objects versus avoiding virtual vacuum excitations. In the multipolar-gauge material systems are fully localised, but if such a “detector” is deemed accessible and is therefore prepared in a particular energetic state, then it will necessarily become excited even within the corresponding photonic vacuum. These virtual excitations are not encountered if one instead deems physical subsystem excitations to be those defined relative to the true ground state of the composite system. This, however, constitutes defining the physical subsystems relative to an unconventional gauge (neither Coulomb nor multipolar). Material systems defined in this way, are necessarily delocalised to some extent. Thus, while in practice a detection process necessarily possesses finite extent in space and time, theoretically some degree of spatial localisation of a detector must be sacrificed if one wishes to eliminate the prediction of its virtual excitation.

The balance between spacetime localisation and the inclusion of virtual quanta becomes significant outside of traditional regimes and is determined by the gauge choice. We review theoretical aspects of cavity QED beyond the weak-coupling regime considering some simple solvable models in this context. We consider virtual excitations in the context of the general theory of weak-measurements.

A. Conventional photodetection theory and its limitations

Glauber photodetection theory [60, 83] has been a major workhorse in weak-coupling quantum optics and constitutes a natural starting point. We briefly review this theory and its limitations.
1. Real excitations

Typical photodetectors work by photon-ionisation amplified to produce a macroscopic current. As such they are substantial objects consisting of photoconductive electrons over a cross-sectional area $S$, that is correlated with detection efficiency. As well as being big, such detectors are also typically slow to respond, at least, compared to the correlation times of the photonic reservoirs that they monitor. Thus, actual photon measurements are not restricted to individual photons in spacetime and this fact is certainly relevant outside of weak-coupling that they monitor. Thus, actual photon measurements with detection efficiency. As well as being big, such detectors are also typically slow to respond, at least, compared to the correlation times of the photonic reservoirs that they monitor. Thus, actual photon measurements are not restricted to individual photons in spacetime and this fact is certainly relevant outside of weak-coupling regimes. However, as a model for dealing with weakly-coupled detectors we may consider a localised “detector” dipole $\mathbf{d} = qr$ fixed at the origin $\mathbf{0}$. The charge $q$ is a suitable perturbation parameter (the fine-structure constant being $\alpha^2/4\pi$).

In each gauge the unperturbed eigenvectors of $H = H_\alpha - V^n$ represent different physical states. Photons are by definition quanta of the “light” subsystem and a detector is a “material” subsystem. A photo-detection process therefore involves an energetic change of the material system, usually accompanied by a change in the number of photons, i.e., it is a process between unperturbed states. Thus, actual photon measurements are not restricted to individual photons in spacetime and this fact is certainly relevant outside of weak-coupling that they monitor. Thus, actual photon measurements with detection efficiency. As well as being big, such detectors are also typically slow to respond, at least, compared to the correlation times of the photonic reservoirs that they monitor. Thus, actual photon measurements are not restricted to individual photons in spacetime and this fact is certainly relevant outside of weak-coupling regimes. However, as a model for dealing with weakly-coupled detectors we may consider a localised “detector” dipole $\mathbf{d} = qr$ fixed at the origin $\mathbf{0}$. The charge $q$ is a suitable perturbation parameter (the fine-structure constant being $\alpha^2/4\pi$).

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In conventional treatments (e.g. Ref. [83]) a linear dipolar form of coupling is adopted as occurs in the multipolar-gauge. This is often written $V^j = -\mathbf{d} \cdot \mathbf{E}_T(\mathbf{0})$ or else $V^j = -\mathbf{d} \cdot \mathbf{E}(\mathbf{0})$. Neither expression is correct. As noted in Sec. II a the correct linear part of the multipolar interaction in the EDA is $V_l = -\mathbf{d} \cdot \mathbf{D}_T(\mathbf{0})$. Two further common misconceptions are that the Coulomb-gauge defines photons using the electric field, and that this is the basic field that first enters into Glauber’s photodetection theory (e.g. Ref. [10]). In fact, the Coulomb-gauge defines photons using $\mathbf{E}_T \neq \mathbf{E}$ and in conventional treatments that employ a dipolar coupling the relevant field entering the theory is correctly identified as $\mathbf{D}_T(\mathbf{0})$. At the dipole’s position $\mathbf{0}$ the field $\mathbf{D}_T$ is infinitely different to $\mathbf{E}(\mathbf{0}) = \mathbf{D}_T(\mathbf{0}) - qr\delta(0)$. However, the infinite term $\mathbf{P}_T(\mathbf{x}) = qr\delta(0)$ is a difference in the source components of the two fields, which are of at least $O(\alpha)$. Since the detector’s dipole moment is of order $q$ only the free (vacuum) component of $\mathbf{D}_T(\mathbf{0})$ contributes to detection probabilities to order $q^2$ in an initially unperturbed state, and this may be taken to coincide with the free component of $\mathbf{E}(\mathbf{0})$.

We begin by following conventional treatments, which define the subsystems photons$_\alpha$ and detector$_\alpha$ relative to the multipolar-gauge $\alpha = 1$, and then employ perturbation theory to order $q^2$. The probability to find the detector excited into the $n$’th level at time $t$, given the initial state $|e^n, \psi_{ph}\rangle$ with a fixed number of photons$_1$ and with $m < n$, is

$$\mathcal{P}^{nm}_d(t) = d_{nm,i} d_{mn,j} \int_0^t ds \int_0^s ds' e^{i\omega_{nm}(s'-s)} G_{ij}(s',s)$$

(233)

where repeated indices are summed, and where

$$G_{ij}(s,s') = \langle \psi_{ph}| E_{vac,i}(s,0) E_{vac,j}(s',0) |\psi_{ph}\rangle$$

(234)

in which

$$E_{vac}(t,\mathbf{x}) = -i \int d^3 k \sum_\lambda \sqrt{\frac{\omega}{2(2\pi)^3}} e_\lambda(k)$$

$$\times \left[ a_\dagger(0,k) e^{i\omega t-i\mathbf{k} \cdot \mathbf{x}} - a_\lambda(0,k) e^{-i\omega t+i\mathbf{k} \cdot \mathbf{x}} \right]$$

(235)

denotes the free component of $\mathbf{D}_T(t,\mathbf{x})$. Since $\omega_{nm} > 0$ the anti-normally ordered contribution in Eq. (233) is taken as rapidly oscillating and is neglected in a rotating-wave approximation (RWA), such that we may let

$$G_{ij}(s,s') = \langle \psi_{ph}| E_{vac,i}(s,0) E_{vac,j}(s',0) |\psi_{ph}\rangle$$

(236)

where

$$E_{vac}(t,0) = i \int d^3 k \sum_\lambda \sqrt{\frac{\omega}{2(2\pi)^3}} e_\lambda(k) a_\lambda(0,k) e^{-i\omega t},$$

$$E_{vac} = (E_{vac}^+)^\dagger.$$  

(237)

We see that normal-ordering occurs as an approximation based on the detector excitation process having a supposedly dominant contribution coming from photon absorption. The neglected contribution is virtual, i.e., number non-conserving, corresponding to detector excitation with emission of a photon$_1$.

The detector level $n$ typically belongs to the ionisation continuum and subsequent to excitation a number of physical processes must occur for a detection event to actually be registered. The description of these processes is subsumed into a classical epistemic probability $\mathcal{P}_n$ for a detection event given excitation to the level $n$. The total probability of detection is therefore

$$\mathcal{P}^n_d(t) = \sum_n \mathcal{P}_n \mathcal{P}^{nm}_d(t)$$

(238)

where formally the summation over $n$ is understood to include integration over continuum levels. Defining the spectral density (sensitivity)

$$S_{ij}(\omega) = 2\pi \sum_n d_{nm,i} d_{mn,j} \delta(\omega - \omega_{nm})$$

(239)

enables one to model different detection schemes by assuming different forms of $S_{ij}(\omega)$. The photon$_1$ counting rate is

$$\frac{d\mathcal{P}^{nm}_d}{dt} = 2Re \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} S_{ij}(\omega) G_{ij}(\omega, t)$$

(240)
where
\[ G_{ij}(\omega, t) = \int_0^t ds \, e^{i\omega(t-s)} G_{ij}(s, t), \]  
(241)
whose Fourier transform is
\[ \mathcal{G}_{ij}(\omega, t) = \int \frac{d\omega}{2\pi} \, e^{i\omega s} G_{ij}(\omega, t) = \theta(s)\theta(t-s)G_{ij}(t-s, t), \]  
(242)
which vanishes unless 0 ≤ s ≤ t. Since photodetectors are slow, the measurement time t is typically much longer than the reservoir correlation time \( T_c = 1/\Delta \omega_G \) where \( \Delta \omega_G \) is the bandwidth of the correlation function \( G_{ij} \). Therefore, the s-width of \( \mathcal{G}_{ij}(s, t) \) is approximately \( T_c \).

Glauber defines an ideal broadband detector as one with a flat spectral density \( S_{ij}(\omega) = S_{ij} \) \cite{83}. This requires that the width of the sensitivity function must be much larger than \( \Delta \omega_G = 1/T_c \), such that \( \mathcal{G}_{ij}(\omega, t) \) is sharply peaked as a function of \( \omega \) when compared with \( S_{ij}(\omega) \). The photon counting rate is then simply \( S_{ij}\mathcal{G}_{ij}(t, t) \) such that if \( S_{ij} \sim \delta_{ij} \) then the rate is proportional to the Glauber intensity
\[ I_G(t) = \left\langle (\mathbf{E}_{\text{vac}}(t, \mathbf{0}) \cdot \mathbf{E}_{\text{vac}}^+(t, \mathbf{0})) \right\rangle. \]  
(243)

2. Virtual excitations

To understand the limitations of this theory we return to Eq. (233). If we assume the vacuum state \( |\psi_{\text{ph}}\rangle = |0\rangle \) and we allow the levels m and n to be arbitrary, then evaluating the polarisation summation and angular integrals gives
\[ \mathcal{P}_{d,\text{vac}}^{mn}(t) = \frac{|d_{mn}|^2}{3\pi} \int_0^\infty d\omega \, \omega^3 \sin^2 \left( \frac{(\omega_{mn} - \omega) t/2}{\pi(\omega_{mn} - \omega)^2/2} \right). \]  
(244)

If \( m > n \) the process described is spontaneous emission. If \( n > m \) then the process described is virtual. The dominant peak of the integrand then lies outside of the domain of integration and is oscillatory for positive frequencies. The amplitude of the oscillations in the integrand grows with \( \omega \) due to the prefactor of \( \omega^3 \). This behaviour is only bounded by an ultra-violet cut-off \( \omega_M \) and the integral is in fact quadratically divergent with \( \omega_M \). The divergence is relatively severe, such that \( \mathcal{P}_{d,\text{vac}}^{mn}(t) \) is non-negligible even for realistic, yet modest values of \( \omega_M \) that are consistent with, for example, the EDA and the non-relativistic treatment [14, 15].

The reason this result occurs is the assumption of an initial unperturbed state consisting of no photons and m excitations of the detector. This state is not an eigenstate of \( H_1 \) and in particular it is not the ground state even if \( m \) is the lowest dipolar level. If this final result is deemed unphysical then we must conclude that the assumed physical states are not operationally relevant in the description of photo-detection, i.e., they cannot be the initial and final states of the relevant physical detector within the relevant photonic environment. If the physical detector is not the localised detector \( 1, \ldots, 15 \), then its physical state is not operationally relevant to the multipolar-gauge, then it must be localised to some extent. The interplay between localisation and dressing is discussed further from Sec. V B onward.

The virtual detection probability \( \mathcal{P}^{mn}_{d,\text{vac}}(t) \) with \( m > n \) is zero in the progression from Eq. (233) to Eq. (240) using the RWA. The counting rate \( d\mathcal{P}^{mn}_{d,\text{vac}}(t)/dt \) without the RWA can be found by direct differentiation of Eq. (244). Subsequently, the virtual rate can again be reduced to zero via the steps that implement Fermi’s golden-rule. This procedure turns the corresponding counting rate into that found using the \( S \)-matrix whereby a real upward detector transition requires real photon absorption. Specifically, differentiation of Eq. (244) yields the frequency integrand \( \omega^3 \sin[(\omega_{mn} - \omega) t]/(\omega_{mn} - \omega) \), which expresses a bare-energy-time uncertainty constraint. Noting that
\[ \lim_{t \to \infty} \frac{\sin(\omega t)}{\pi \omega} = \delta(\omega), \]  
(245)
we see that the limit \( t \to \infty \) imposes strict bare-energy conservation as in the \( S \)-matrix. In this case, if \( n > m \) then since \( \omega_{mn} \) and \( \omega \) have opposite sign the rate \( d\mathcal{P}^{mn}_{d,\text{vac}}(t)/dt \) vanishes. Similarly, if \( m > n \) then we obtain a time-independent rate \( d\mathcal{P}^{mn}_{d,\text{vac}}(t)/dt = \omega_{mn}^3 |d_{mn}|^2/(3\pi) =: \Gamma_{mn} \) which is nothing but the Fermi golden-rule spontaneous emission rate for the downward transition \( m \to n \).

Exactly the same results can be obtained by instead defining the counting rate as the difference quotient \( (\mathcal{P}^{mn}_{d,\text{vac}}(t) - \mathcal{P}^{mn}_{d,\text{vac}}(0))/t = \mathcal{P}^{mn}_{d,\text{vac}}(t)/t \). From Eq. (244) this definition yields the frequency integrand \( \omega^3 \sin^2[(\omega_{mn} - \omega) t]/[\omega_{mn} - \omega]^2 t/2) \), whose long-time limit is found using
\[ \lim_{t \to \infty} \frac{\sin^2(\omega t/2)}{\pi \omega^2 t/2} = \delta(\omega). \]  
(246)

Thus, in the limit \( t \to \infty \), for \( n > m \) we again find that the rate vanishes while for \( n \leq m \) we again obtain the rate \( d\mathcal{P}^{mn}_{d,\text{vac}}(t)/dt = \omega_{mn}^3 |d_{mn}|^2/(3\pi) =: \Gamma_{mn} \). On the other hand the derivative \( d\mathcal{P}^{mn}_{d,\text{vac}}(t)/dt \) is strictly recovered on the left-hand-side via the limit \( t \to 0 \). This shows that the overall procedure for obtaining \( \Gamma_{mn} \) constitutes a form of Markov approximation which consecutively employs limits \( t \to 0 \) and \( t \to \infty \) and therefore requires a clear separation of time scales. The procedure should be valid for real emission with rate \( \Gamma_{mn} \) within the Markovian regime
\[ \frac{1}{\omega_{mn}} \ll t \ll \frac{1}{\Gamma_{mn}} \]  
(247)
provided that matrix elements of the interaction Hamiltonian between initial and final states are
sufficiently small and slowly varying. To see this note that a third method of obtaining the rate \( \Gamma_{mn} \) for \( m > n \) is to evaluate the prefactor \( \omega^3 \) in Eq. (244) on resonance \( \omega = \omega_{mn} \), which is valid if it can be considered sufficiently slowly varying compared with the peak in 
\[
\sin^2[\omega_{mn} - \omega]t/(\omega_{mn} - \omega)^2 t/2 \]
which lies outside of the range of integration and the integral diverges because as already noted the dominant peak in
\[
\sin^2[\omega_{mn} - \omega]t/(\omega_{mn} - \omega)^2 t/2 \]
One then extends the lower integration limit to \(-\infty\) by supposing that the remaining integrand is dominated by this peak for sufficiently long times \( \omega_M t \gg 1 \). It is not clear that this same procedure can be justified for virtual excitation with \( n > m \), because as already noted the dominant peak in
\[
\sin^2[\omega_{mn} - \omega]t/(\omega_{mn} - \omega)^2 t/2 \]
then lies outside of the range of integration and the integral diverges quadratically with \( \omega_M \). In this sense virtual contributions are non-Markovian.

So far we have considered only the detector1 and light1 subsystems and yet the severity of the divergence in \( \mathcal{P}_{nm, \text{d,vac}}(t) \) that we have found is indeed specific to these subsystems. It results from the interaction \( V^1 \) possessing a factor \( \sqrt{\omega} \), which comes from the mode expansion of \( \mathbf{D}_T(0) \) in Eq. (235). This results in the prefactor \( \omega^3 \) in the integrand of Eq. (244). A detector that is defined relative to a different gauge is a different physical detector and therefore it possesses different physical predictions; the field entering into the theory is not \( \mathbf{D}_T(0) \).

We note that as in the textbook [84] the actual field involved in the theory can be left open by defining

\[
\mathbf{F}(t, \mathbf{x}) = \int \frac{d^3 k}{\sqrt{2}(2\pi)^3} \sum_\lambda \mathbf{e}_\lambda(k)\beta(\omega) a_\lambda(t, k)e^{ik\cdot x} \tag{248}
\]

where a number of noteworthy choices of \( \beta(\omega) \) can be made. For example, if \( \beta(\omega) = 1/\sqrt{\omega} \) then \( \mathbf{F} = \mathbf{D}_T \). If \( \beta(\omega) = 1/\sqrt{\omega} \) then \( \mathbf{F} = \mathbf{A}_T \). If \( \beta(\omega) = 1 \) then \( \mathbf{F}^{(+) = \mathbf{F}^{(-)} \circ \mathbf{F}^{(+)}(\mathbf{x}) \circ \mathbf{F}^{(+)}(\mathbf{x}) \) can be interpreted as a real-space number density of photons that are approximately localised on a scale much larger than the corresponding wavelengths [84] (see also Sec. V C 1). We remark that being local in \( k \)-space, the relation between fields corresponding to different \( \beta(\omega) \) in Eq. (248) is highly non-local in spacetime. This point is relevant to understanding the interplay between electromagnetic dressing and localisation and is discussed further in Sec. V C.

It is instructive to repeat the derivation of the detector excitation rate for a detector0, i.e., for a detector defined relative to the Coulomb-gauge. The linear interaction is then \( V^0 = -q\mathbf{p} \cdot \mathbf{A}_T(0)/m \) where as before we can neglect order \( q^2 \) components of the interaction. The basic field entering into the theory is now \( \mathbf{A}_T(0) \) and the final result amounts to letting \( \beta(\omega) = 1/\sqrt{\omega} \) in Eq. (248). In place of Eq. (244) we obtain

\[
\mathcal{P}_{nm, \text{d,vac}}(t) = \frac{d_{nm}^2}{3\pi^2} \int_0^{\infty} d\omega \omega_{mn}^2 \frac{\sin^2[\omega_{mn} - \omega]t/2}{\pi(\omega_{mn} - \omega)^2 / 2}. \tag{249}
\]

Using the Markov approximation, i.e., using Fermi’s golden-rule, we obtain \( d\mathcal{P}_{nm, \text{d,vac}}/dt = \Gamma_{mn} \) for \( m > n \) and \( d\mathcal{P}_{nm, \text{d,vac}}/dt = 0 \) for \( n > m \), exactly as was obtained for the (physically distinct) detector and light1 subsystems. This is a direct demonstration of the non-occurrence of subsystem gauge-relativity within the S-matrix, as described in Sec. IV A.

Without the Markovian approximation the probabilities in Eqs. (244) and (249) are clearly different. However, both are gauge-invariant as implied by Eq. (177). More precisely, for initial and final unperturbed states represented by vectors \( |e^m, \phi_{ph}\rangle \) and \( |e^n, \psi_{ph}\rangle \) respectively, we obtain for the subsystems defined relative to the gauge \( \alpha \) the probability \( \mathcal{P}_\alpha(t) = \langle e^m, \phi_{ph}| U_{\alpha}(t, 0)| e^n, \psi_{ph}\rangle \). The same physical prediction is calculated in the gauge \( \alpha' \) by noting that the same initial and final physical states are represented by vectors \( |e^m, \psi_{ph}\rangle = R_{\alpha\alpha'}|e^m, \psi_{ph}\rangle \) and \( |e^n, \phi_{ph}\rangle = R_{\alpha\alpha'}|e^n, \phi_{ph}\rangle \) respectively, while the physical evolution is provided by \( U_{\alpha'}(t, 0) = R_{\alpha\alpha'} U_{\alpha}(t, 0) R_{\alpha\alpha'}^\dagger \). Thus, as noted in Sec. IV A, finite-time predictions such as \( \mathcal{P}_\alpha(t) \) are necessarily gauge-invariant for every value of \( \alpha \), a fact guaranteed by the unitarity of gauge-fixing transformations. However, as also noted in Sec. IV A, outside of weak-coupling and Markovian regimes, it must be recognised that \( \mathcal{P}_\alpha(t) \) constitutes a different gauge-invariant prediction for each different \( \alpha \).

In comparing specifically the different physical predictions given by Eqs. (244) and (249), Power and Thirunamachandran have noted that which one is the more accurate will depend on which set of distinct physical states represented by the same unperturbed vectors within the two gauges, are closer to the states actually realised in the considered experiment [28, 29]. Power and Thirunamachandran also noted that experiments could be used to determine which descriptions are most appropriate.

When \( n > m \), the probability for the detector0 in Eq. (249) is only logarithmically divergent and is therefore significantly different to the corresponding detector1 prediction in Eq. (244). This much less severe divergence is a direct consequence of the \( k \)-space normalisation of the field \( \mathbf{A}_T \), which is \( 1/\sqrt{\omega} \). We note that in any gauge, if the RWA is avoided and the broadband limit is taken then the photon counting rate is \( S_{ij} G_{ij}(t, t) \) with \( G_{ij}(t, t) \) given by Eq. (236) rather than Eq. (242). Thus, a generally large virtual contribution occurs. However, the broadband limit is inapplicable to this contribution because the vacuum has infinite bandwidth. Thus, the significance of such contributions is in general dependent on the measurement schemes available.

The elimination of divergent contributions requires “renormalisation” of the “bare” dipole by defining the
“physical” dipole relative to the appropriate gauge as recognised some time ago by Drummond [15]. One can use the elimination of virtual excitations as a criterion by which to select the most operationally relevant subsystem definitions, that is, to select the most appropriate gauge relative to which the dipole is to be defined in the context of photodetection. To show how this can be achieved we consider a one-dimensional dipole harmonically quantised in the direction \( \hat{u} \) with canonical operators

\[
\mathbf{r} = \frac{\hat{u}}{\sqrt{2m\omega_m}} (b^\dagger + b), \tag{250}
\]

\[
\mathbf{p} = i\hat{u} \sqrt{\frac{m\omega_m}{2}} (b^\dagger - b). \tag{251}
\]

From very early on purely bosonic models of this kind have been relevant to ultrastrong-coupling in polaritonic systems with quantum wells and microcavities [64–67].

We consider gauges of the form specified by Eq. (81) while assuming that \( \alpha(k) = \alpha(\omega) \) is real and depends only on the magnitude of \( \mathbf{k} \). Thus, here we are going to exploit the possibility of gauge functions that vary with the mode argument \( \mathbf{k} \), of which the Coulomb and multipolar gauges \( \alpha(k) = 0,1 \) are not examples. We discretise the Fourier modes within a volume \( v \) and combine wavevector and polarisation indices into a single mode label, writing \( \alpha(\omega) = \alpha_k \). The polarisation self-energy term \( \int d^3x P_{tg}^2 \) can be absorbed via new material modes such that

\[
\mathbf{r} = \frac{\hat{u}}{\sqrt{2m\omega_m}} (d^\dagger + d) \tag{252}
\]

\[
\mathbf{p} = i\hat{u} \sqrt{\frac{m\omega_m}{2}} (d^\dagger - d). \tag{253}
\]

where

\[
\tilde{\omega}_m^2 = \omega_m^2 + \frac{q^2}{m!} \sum_k (e_k \cdot \hat{u})^2 \alpha_k^2. \tag{254}
\]

Similarly, the order \( q^2 \) field self-energy term \( q^2 (\mathbf{A}_g^2)^2 / (2m) \) can be absorbed via radiative mode operators \( c_k \) such that

\[
a_k = \sum_j \left( [\cosh \theta]_{kj} c_j + [\sinh \theta]_{kj} c_j^\dagger \right)
\approx c_k + \sum_j \theta_{kj} c_j^\dagger \tag{255}
\]

where the approximate equality holds to order \( q^2 \) because \( \theta \) is an \( \alpha_k \)-dependent symmetric matrix of order \( q^2 \) defined by

\[
\theta_{kj} = -\frac{q^2}{2m} \frac{e_k \cdot e_j (1 - \alpha_k)(1 - \alpha_j)}{\sqrt{\omega_k \omega_j (\omega_k + \omega_j)}}. \tag{256}
\]

The arbitrary-gauge Hamiltonian can now be written correct to order \( q^2 \) as

\[
H_g = \tilde{\omega}_m \left( d^\dagger d + \frac{1}{2} \right) + \sum_{k,j} \omega_{kj} \left( c_k^\dagger c_j + \delta_{kj} \frac{1}{2} \right)
- \frac{q}{m} \mathbf{p} \cdot \mathbf{A}_g(0) + q \mathbf{r} \cdot \mathbf{\Pi}_g(0) \tag{257}
\]

where

\[
\omega_{kj} = \omega_k \delta_{kj} + (\omega_k + \omega_j) \theta_{kj} \tag{258}
\]

and

\[
\mathbf{A}_g(0) := \sum_{k,j} \frac{e_k}{\sqrt{2\omega_k v}} (1 - \alpha_k) [e_j^\dagger c_j + c_j], \tag{259}
\]

\[
\mathbf{\Pi}_g(0) := i \sum_{k,j} e_k \sqrt{\frac{\omega_k}{2v}} \alpha_k [e^{-\omega} c_j - c_j^\dagger]. \tag{260}
\]

Since the linear interaction components in Eq. (257) are of order \( q \) we may let \( [e^\omega]_{kj} = \delta_{kj} \) in the mode expansions (259) and (260) to obtain results correct to order \( q^2 \), amounting to the straightforward replacement \( a_k \rightarrow c_k \) within the interaction Hamiltonian. Similarly, when used within the interaction Hamiltonian we may let \( \tilde{\omega}_m = \omega_m \) in the expansions (252) and (253), amounting to the replacement \( b \rightarrow d \). We remark that the renormalisation of self-terms is consistent with an interpretation in which bare frequencies are not viewed as physical. This renormalisation does not affect the choice of gauge or the subsystem partition.

The results above that assumed linear multipolar- and Coulomb-gauge interactions from the outset remain applicable. Although the renormalised frequencies contain order \( q^2 \) contributions, the detectors excitation at time \( t \) is already at least of order \( q^2 \), so the renormalised frequencies should be approximated as bare. Assuming the initial state \( |0,0\rangle \) with no photons and no initial detector excitation we calculate the average detector population as

\[
\langle d^\dagger(t) d(t) \rangle_{0,d,v} = \Gamma \int_0^\infty d\omega \left[ \frac{\omega u^+(\omega) \sin [\tilde{\omega}_m + \omega] t}{\omega \tilde{\omega}_m} \right]^2 \tag{261}
\]

where \( \Gamma = q^2 \omega_m^2 / (6m^2) \) is the total oscillator spontaneous emission rate into the ground state and where

\[
u^+(\omega) = \sqrt{\frac{\omega_m}{\omega}} \left( 1 - \alpha(\omega) \right) - \frac{\omega - \omega_m}{\omega_m} \alpha(\omega) \right). \tag{262}
\]

The multipolar- and Coulomb-gauge cases are given by \( \alpha(\omega) = 1 \) and \( \alpha(\omega) = 0 \) respectively. The results for these gauges can also be found using the formula

\[
\langle d^\dagger(t) d(t) \rangle_{0,d,v} = \sum_n \mathcal{P}_{n,d,v}(t) \text{ with } \mathcal{P}_{n,d,v}(t) \text{ given by Eqs. (244) and (249) respectively. The rate}
\]

\[
\frac{d}{dt} \langle d^\dagger(t) d(t) \rangle_{0,d,v}
= \frac{\Gamma}{\pi} \int_0^\infty d\omega \frac{\omega_m^2 u^+(\omega)^2 \sin [\tilde{\omega}_m + \omega] t}{(\omega_m + \omega)} \tag{263}
\]
is highly oscillatory. As already noted the integrand averages to zero in the long-time limit $t \rightarrow \infty$, while for finite times $1 \ll \omega_m t \ll \omega_m/T$ the Markovian approximation is not necessarily applicable.

The rapid oscillations in the detector’s excitation can be removed to reveal the averaged behaviour by considering the time-average over an interval $T \gg 1/\omega_m$, defined by

$$R = \frac{1}{T} \int_0^T dt \frac{d}{dt}(d^\dagger(t)d(t))_{0_\alpha,0_\alpha} = \frac{1}{T}(d^\dagger(t)d(t))_{0_\alpha,0_\alpha}$$

$$= \frac{\Gamma}{\pi T} \int_0^\infty d\omega \left[ \frac{\omega u^+(\omega)}{\omega_m(\omega_m + \omega)} \right]^2$$

(264)

where we have replaced $\sin^2 [(\omega_m + \omega)T]/2$ in Eq. (261) by its average $1/2$ for $\omega_m T \gg 1$. The Coulomb and multipolar-gauge time-averaged rates are plotted in Fig. 7. The multipolar rate in particular is quadratically divergent with $\omega_M$ whereas the Coulomb-gauge rate is logarithmically divergent.

However, if we choose $\alpha = \omega_m/(\omega_m + \omega_k)$ [cf. Eq. (190)] then we obtain the Hamiltonian [cf. Eq. (196)]

$$H_{JC} = \bar{\omega}_m \left( d^\dagger d + \frac{1}{2} \right) + \sum_{k,j} \omega_{kj} \left( c_k^\dagger c_j + \frac{\delta_{kj}}{2} \right)$$

$$- i q \sum_k \sqrt{\frac{\omega_k \omega_m}{mv}} \frac{1}{\omega_m + \omega_k} (d^\dagger c_k - dc_k^\dagger).$$

(265)

In this gauge the ground state is represented by the vector $|0_d,0_\alpha\rangle$ annihilated by $d$ and $c_k$. It is easy to verify that the ground energy eigenvalue of $H_{JC}$ produces the expected order $q^2$ ground state Lamb shift [15]. In this gauge the detector excitation rate is identically zero because $u^+(\omega) \equiv 0$.

3. Discussion

Subsystems defined relative to the JC-gauge are such that detector excitations and photons are excitations relative to the true ground state of the interacting system. This however, does not require a full diagonalisation of the dipolar Hamiltonian, instead it requires only separate (non-mixing) light and matter transformations within the selected JC-gauge. While the ground state of the composite system can of course be identified in any gauge, it is only within the JC-gauge that this state coincides with the ground state of the subsystems. Thus, if this property were proposed as a criterion by which to identify the most physically relevant subsystems, then said subsystems are not those defined relative to any conventional gauge. Conversely, spatial localisation may be deemed the relevant figure of merit in defining the physical detector subsystem. In particular, the multipolar-gauge detector, constitutes a fully localised detector, but also one for which the divergence in virtual detector excitation was most severe.

In summary, we have seen that virtual processes occurring in photodetection are non-Markovian and strongly gauge-relative. They are not necessarily negligible even within the weak-coupling regime. Their suppression can be invoked as a criterion by which to identify the gauge relative to which the most physically relevant subsystems are to be identified. Their contributions are also suppressed by weak-coupling “approximations”, which mimic the $S$-matrix and enforce bare-energy conservation (cf. Sec IV B) despite not necessarily being applicable. In what follows, we focus on effects outside of the standard weak-coupling approximations, which we expect to be especially significant in strong and ultrastrong-coupling regimes. We will see that if a detector is by definition localised, then outside of weak-coupling and Markovian regimes such a detector necessarily experiences virtual vacuum excitations.

B. Localisation and causality

1. Electromagnetic source-fields in an arbitrary gauge

To understand photodetection outside of the standard quantum optics paradigm it will be necessary to determine the electromagnetic fields generated by a source in an arbitrary gauge. In particular, if we consider a system consisting of both a source $s$ and detector $d$ then the total electric field is a superposition of vacuum, source, and detector fields;

$$E = E_{vac} + E_s + E_d.$$ 

(266)

However, a full description of the source-detector-field system is postponed until Sec. V B 2. First we note that due to subsystem gauge-relativity the partitioning of a gauge-invariant field into vacuum, source, and detector...
components, is gauge-relative [28, 29]. In other words, while the left-hand-side of Eq. (266) is unique, the individual components on the right-hand-side represent different physical fields in different gauges. We therefore start by considering only one material system; a point dipole fixed at \( 0 \) and with dipole moment \( qr \). For simplicity, we again restrict our attention to the one-parameter \( \alpha \)-gauge framework.

Let us consider the canonical field \( \Pi \) at an arbitrary point \( x \neq 0 \), which can be partitioned as

\[
\Pi(t, x) = -E_T(t, x) - \alpha E_L(t, x) = \Pi_{\text{vac}}^\alpha(t, x) + \Pi^\alpha_x(t, x). \tag{267}
\]

In the gauge \( \alpha \) the vacuum and source components \( \Pi_{\text{vac}}^\alpha(t, x) \) and \( \Pi^\alpha_x(t, x) \) are defined as the components whose dynamics are generated by \( H_{\text{ph}} \) and \( V^\alpha \) respectively. The vacuum field is defined by the right-hand-side of Eq. (235). Since the photons defined by \( a_\lambda(0, k) \) are physically distinct for each \( \alpha \) the vacuum field depends on \( \alpha \). The source field obviously depends on \( \alpha \) and the dynamics generated by \( H_\alpha = H_m + H_{\text{ph}} + V^\alpha \) yield

\[
\Pi^\alpha_x(t, x) = -\theta(t_r)X_T(t_r, x) + (1 - \alpha)\left[ P_T(t, x) - \theta(-t_r)P_T(0, x) \right] \tag{268}
\]

where \( t_r = t - x \) is the retarded time (in units with \( c = 1 \)) in which \( x = |x| \) is the distance from the dipole source at \( 0 \) and where for \( x \neq 0 \)

\[
X_{T, i}(t_r, x) = \left( -\partial^2 \delta_{ij} + \partial_i \partial_j \right) \frac{qr_j(t_r)}{4\pi x}. \tag{269}
\]

Note that the derivative operators in Eq. (269) act on \( t_r \) as well as on \( 1/x \). Only the top line on the right-hand-side of Eq. (268) is causal, by which we mean vanishing for \( t_r < 0 \), and the second line only vanishes for \( \alpha = 1 \).

Using the fact that the \( a_\lambda(0, k) \) of different gauges are related by \( R_{a\alpha'} \), one finds that the different vacuum components \( \Pi_{\text{vac}}^\alpha \) are related by

\[
\Pi_{\text{vac}}^\alpha(t, x) = \Pi_{\text{vac}}^{\alpha'}(t, x) - (\alpha - \alpha')\theta(-t_r)P_T(0, x). \tag{270}
\]

It follows that the combination \( \Pi_{\text{vac}}^\alpha(t, x) + \alpha\theta(-t_r)P_T(0, x) \) is actually \( \alpha \)-independent. We see also that for different \( \alpha \) the vacuum components \( \Pi_{\text{vac}}^\alpha \) differ by an \( \alpha - \alpha' \) weighted factor of \( P_T = E_L \) evaluated at \( t = 0 \), and that this contribution is restricted to the complement of the interior lightcone of the origin \((0, 0)\) of the dipole’s rest-frame. This is an expression of subsystem gauge-relativity, that is, from the outset the definition of material source differs between gauges in the extent to which the electrostatic field \( P_T = E_L \) is included.

It is instructive to consider some specific physical fields. For example, \( E_T = -\Pi_{\alpha=0} \) for which \( E_{Ta} = -\Pi^\alpha_a - \alpha P_T \) and \( E_{T_{\text{vac}}} = -\Pi_{\text{vac}}^\alpha \). Clearly the free and source components are different in different gauges, but their sum is

\[
E_T(t, x) = \theta(t_r)X_T(t_r, x) + \theta(-t_r)P_T(0, x) - P_T(t, x) - \Pi_{\text{vac}}^\alpha(t, x) - \alpha\theta(-t_r)P_T(0, x) \tag{271}
\]

which upon taking into account Eq. (270) is seen to be unique (\( \alpha \)-independent) as required. The total electric field is for \( x \neq 0 \) given by \( E = D_T = -\Pi_{\alpha=1} = E_P + P_T \), which can be read-off immediately from Eq. (271) as

\[
E(t, x) = D_T(t, x) = \theta(t_r)X_T(t_r, x) + \theta(-t_r)P_T(0, x) - \Pi_{\text{vac}}^\alpha(t, x) - \alpha\theta(-t_r)P_T(0, x). \tag{272}
\]

Similarly to Sec. II H, the results above demonstrate that what differs for different choices of \( \alpha \) are the localisation properties of the source. For \( t_r > 0 \), we have that \( E_s(t, x) = D_{Ta}(t, x) = X_T(t_r, x) \) and \( E_{Ta}(t, x) = X_T(t_r, x) - P_T(t, x) \) for all \( \alpha \). In words, at all points \( x \) that can be connected to the source’s centre by a light signal emitted a time \( x \) earlier, each physical field’s source component is independent of the source’s definition. In contrast, for \( t_r < 0 \) the source-vacuum partitioning of a given physical field differs between different gauges \( \alpha \).

For any \( \alpha \) the source component \( E_{Ta}^\alpha(t, x) \) is non-zero for \( t_r < 0 \), due to the non-vanishing \( \alpha \)-independent term \( -P_T = -E_L \) in Eq. (271). The total electric field is obtained by adding \( E_L \) to \( E_T \) in Eq. (271), which removes this instantaneous component, yielding Eq. (272). However, this does not imply that the electric field \( E_{Ta}^\alpha(t, x) \) vanishes for \( t_r < 0 \) unless we also insist that the source itself is also fully localised, i.e., unless we define the source relative to the multipolar-gauge. As explained in Sec. II H, the gauge controls the extent to which the instantaneous field \( E_L = P_T \) is included within the source’s definition. The gauges \( \alpha = 0 \) and \( \alpha = 1 \) are extremal cases whereby \( E_L \) is fully included and completely absent respectively. For this reason, when \( t_r < 0 \) Eq. (272) reads \( E(t, x) = -\Pi_{\text{vac}}^\alpha(t, x) + (1 - \alpha)P_T(0, x) \), such that only in the multipolar-gauge \( \alpha = 0 \) do we obtain \( E(t, x) = -\Pi_{\text{vac}}^\alpha(t, x) \) and therefore \( E_{Ta}^\alpha(t, x) = 0 \).

More generally, the source-component of the field \( \Pi = -E_T - \alpha'P_T \), when partitioned according to the gauge \( \alpha \) to give \( \Pi^\alpha = -E_{Ta}^\alpha - \alpha'P_T \), is causal (meaning vanishing for \( t_r < 0 \), if and only if \( \alpha = 1 \) and \( \alpha' = 1 \). The latter equality \( \alpha' = 1 \) specifies that the physical field being considered is \( E \), which is a local field, and the former equality \( \alpha = 1 \) specifies that the source producing this field is defined relative to the multipolar-gauge, and is therefore itself also local.

In contrast to the electric field, it is easy to show that unlike \( E \) the magnetic field \( B = B_{\text{vac}} + B_\alpha \) has unique vacuum and source components and that \( B_\alpha \) is causal [29]. These results generalise those of Ref. [29] by giving vacuum-source partitions of the physically arbitrary field \( \Pi \), using an arbitrary gauge \( \alpha \). For any given physical field the relative magnitude of the non-local contributions occurring for \( t_r < 0 \) vary with \( \alpha \) and provide a measure.
of the delocalisation of the source, as will be elaborated further below and in Sec. V C 2.

2. Source-detector-field system

Let us now consider the tripartite source-detector-field system. If we require the detector dipole to be fully localised at $x$ and a source dipole to be fully localised at $0$, then “matter” must be defined relative to the multipolar-gauge. From the results of Sec. V B 1 it is also clear that the response of the detector to the source it is to be causal. This follows from Hegerfeldt’s theorem, which is a general mathematical result that assumes i) the energy is bounded from below, ii) the source and detector are initially localised in disjoint regions, iii) the initial state consists of the source excited and the detector in its ground state with no photons present [61]. Hegerfeldt showed that under these assumptions, the total probability of excitation of the detector, $\mathcal{P}_d(t) = \mathcal{P}_{d,0}(t) + \mathcal{P}_{d,s}(t)$, is either necessarily non-zero for times $t < 0$, or that it is identically zero for all times. It follows that for an initial state represented by the vector $|\epsilon^d_+, \epsilon^d_0)\rangle$ in the multipolar gauge, if $\mathcal{P}_{d,0}(t)$ were to vanish, then $\mathcal{P}_{d,s}(t)$ would be non-zero for $t < 0$ and this would violate Einstein causality, because the multipolar-gauge dipoles are localised and spacelike separated.

By assuming the initial state $|\epsilon^s_n, \epsilon^d_0)\rangle$ in the multipolar-gauge one is assuming that the bare multipolar-gauge dipoles are those that are operationally relevant at the preparation stage, but since $|\epsilon^d_0)\rangle$ is not the ground state of the detector-field system this leads to the immediate virtual excitation of the detector for $t > 0$. We have seen that this virtual excitation is actually necessary to preserve Einstein causality. Hegerfeldt also notes however, that like a violation of Einstein causality, such virtual (spontaneous) excitations are themselves conceptually problematic and are essentially what one seeks to eliminate within a successfully renormalised theory. Indeed, we saw in Sec. V A that the multipolar dipole’s virtual excitation was particularly unphysical and we identified a different gauge within which such excitations were eliminated. In any such theory the detector responds to the source for times $t_r < 0$. To avoid
a conflict with Einstein causality one must interpret the renormalised source and detector as objects that are delocalised around their centres at $0$ and $R_i$ respectively.

The representation in which virtual excitations are removed is one in which the initial state of the detector and field subsystems coincides with the detector-field ground state, which might be considered a more realistic initial state. Predictions for this situation will be given in Sec. V C 2. However, this state cannot be prepared independent of the source and so is clearly delocalised. Since preparation and measurement procedures necessarily possess finite extent in spacetime, there is clearly a balance to be struck between dressing and localisation. The parameter $\alpha$ affects this balance by controlling the extent to which bare matter is dressed by $\alpha$, balance to be struck between dressing and localisation.

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Thus, in this regime it is possible to define the detector dipole as a localised system, while also retaining a fully causal response to the source, but without spontaneous vacuum excitation. This combination of properties is forbidden by Hegerfeldt’s theorem and must therefore be the culmination of weak-coupling approximations. In sufficiently strong-coupling regimes one or more of these properties must be sacrificed. The gauge $\alpha$ relative to which the detector is defined will affect which properties of its weak-coupling counterpart it continues to possess. The multipolar gauge continues to define localised dipoles with causal interactions, but with $\mathcal{P}_{d,0}(t) \neq 0$. On the other hand values $\alpha \neq 1$ define dipoles that are delocalised to some extent, but which may retain the property $\mathcal{P}_{d,0}(t) \approx 0$ even outside of the weak-coupling regime.

C. Local densities

1. Non-local connections between free photonic fields

Relativistic quanta such as photons do not possess a position operator and cannot be localised [84–86]. Quadratic functions of $E$ and $B$ such as the energy-density and Poynting vector, are local, but have the dimensions of energy-density rather than number density. We noted in Sec. V A that distinct gauge-invariant fields $A_T$ and $D_T$ were relevant in photodetection for subsystems defined relative to the Coulomb and multipolar-
gauges respectively, and we noted that both of these fields are special cases of Eq. (248). Before calculating average values of local energy-densities we briefly review the connection between some examples of fields defined by Eq. (248) for different $\beta(\omega)$. We first consider free electrodynamics (no charges).

There are several commonly encountered operations performed on the local fields $E$ and $B$, which are local in $k$-space and therefore non-local in spacetime. Specifically, $i)$ the longitudinal and transverse projection of a local field is non-local; $ii)$ the projection of a local field onto its positive and negative frequency components is non-local in time. Moreover, causal wave propagation requires both signs of the frequency [85], so the positive and negative frequency components of a causal field are only themselves causal within the Markovian approximation of extending frequency integrals over the whole real line [26, 89]: $iii)$ the (arbitrary-gauge) fields defined by Eq. (248) corresponding to different choices of $\beta(\omega)$ are non-locally connected.

To exemplify point $iii)$ note that the Glauber intensity is non-locally connected to the naive “photon number density” $\mathbf{V}^{(+)}$, $\mathbf{V}^{(+)}$ defined by [84]

$$\mathbf{V}^{(+)}(t, x) = \int \frac{d^3k}{(2\pi)^3} \sum_{\lambda} e_{\lambda}(k) a^\dagger_A(k) e^{ik \cdot x - i\omega t} \quad (277)$$

$$= \int d^3k \sqrt{\omega} e^{ik \cdot x} = \frac{3}{8\sqrt{2\pi^3}x^3} \quad (278)$$

Because of this, if a single photon were to be considered localised around $0$, then its energy would be less localised, falling off as $x^{-7}$ [84]. Similarly, the fields $\mathbf{A}^{(+)}$ and $\mathbf{B}^{(+)}$ are related in $k$-space by a factor of $\omega$, so the relevant kernel is

$$K(x) = \int \frac{d^3k}{(2\pi)^3} \omega e^{ik \cdot x} = \frac{1}{\pi^2 x^4} \quad (280)$$

Given the non-local connections between free photonic fields corresponding to different $\beta(\omega)$ in Eq. (248) it is unsurprising that the inclusion of virtual photons within the definition of a source requires non-local operations in spacetime. Further understanding is gained by analysing local energy-densities in the presence of the source, as reviewed below.

2. Second-order energy-densities

In order to understand the interplay between local fields, virtual processes, and subsystem gauge-relativity, we now consider various energy-densities in the vicinity of a dipole [17, 28, 29, 45, 54–57, 89–93]. In finding energy-densities different methods are available and are suitable for different purposes. For a two-level dipole, energy-densities can be found without resorting to perturbative expansion of the electromagnetic fields by instead...
using the rotating-wave and Markov approximations. The RWA imposes number conservation and thereby restricts to processes for which the Markov approximation $\sigma^{\pm}(s) \approx \sigma_{\pm}(t)e^{\pm i\omega_{m}(s-t)}$, $0 \leq s \leq t$, can subsequently be applied when calculating canonical photonic fields. Combined with the extension of frequency integrals over the whole real line the overall result of these approximations is to enforce strict bare-energy conservation. This description captures the exponential decay of excited states, but causes virtual contributions to vanish identically.

To describe virtual contributions we evaluate expressions perturbatively, which does not imply a lower bound on the time-scales described. In this case, in all expressions that are second order in $q$ one approximates the photonic and dipolar operators at times $s \in [0, t]$ as freely evolving within the interaction picture [56, 91]. This does not capture the exponential decay of excited states, but it can be seen to be consistent with the non-perturbative approach applicable to a two-level dipole. Specifically, if negative frequencies are included as a form of Markov approximation, then only real contributions remain and for a two-level dipole the results obtained coincide with the short-time limit of the non-perturbative results found using the rotating-wave and Markov approximations.

First we take the multipolar-gauge bare state $|\epsilon^{p}, 0\rangle$ where $p$ is arbitrary, as the initial state and use the multipolar-gauge interaction $V^{1} = \mathbf{d} \cdot \mathbf{\Pi}(0)$, $\mathbf{d} = q \mathbf{r}$. The second order interaction $\int d^{3}x P_{\mathbf{x}}(x) \mathbf{d}^{2}/2$ can be ignored for predictions up to order $q^{2}$. The electric and magnetic fields are expanded up to order $q^{2}$ for $x \neq 0$:

$$
\mathbf{E} = \mathbf{D}_{T} = \mathbf{E}_{\text{vac}} + \mathbf{E}_{1} + \mathbf{E}_{2},
$$

$$
\mathbf{B} = \mathbf{B}_{\text{vac}} + \mathbf{B}_{1} + \mathbf{B}_{2}.
$$

(281)

(282)

Recall that, as discussed in Sec. V B 1, the partitioning of the electric field into vacuum and source fields is gauge-relative, so the components on the right-hand-side of Eq. (281) must be understood as being specific to the multipolar-gauge (they are generated by interaction $V^{1}$). The first and second order (source) fields are

$$
E_{1,i}(t, x) = \frac{\theta(t_{r})}{4\pi} \sum_{l,n} |\epsilon^{n}\rangle \langle \epsilon^{l}| \frac{d_{il}}{d_{nl}} \omega_{nl} f_{ij}(\omega_{nl}x)e^{-i\omega_{nl}t_{r}}
$$

$$
E_{2,i}^{(\pm)}(t, x) = \frac{i\theta(t_{r})}{4\pi} \sum_{k\lambda} \sqrt{\frac{\omega}{2\pi}} \sum_{l,n,p} |\epsilon^{p}\rangle \langle \epsilon^{l}| a_{k\lambda} e^{ik\lambda} \left[ \left( \frac{d_{in}^{\dagger}d_{np}^{} + d_{in}^{\dagger}d_{np}^{} - d_{in}^{\dagger}d_{np}^{} \omega_{np} - \omega}{\omega_{nl} + \omega} \right)^{3} \omega_{np} f_{ij}(\omega_{np} + \omega)x^{l}(\omega_{np} - \omega)_{r} 
\right.

- \left. d_{in}^{\dagger}d_{np}^{} \omega_{nl} f_{ij}(\omega_{nl}x)e^{i\omega_{nl}t_{r}} 
\right]

$$

(283)

(284)

where the modes have been discretised in a volume $v$. The magnetic counterparts are given by the same expressions with $f_{ij}$ replaced by $g_{ij}$. These tensor components are defined by

$$
f_{ij}(\omega x) := \frac{\theta(t_{r})}{\omega_{x}} + \phi_{ij} \left( \frac{-i}{\omega_{x}} + \frac{1}{(\omega_{x})^{3}} \right),
$$

$$
g_{ij}(\omega x) := \varphi_{ij} \left( \frac{1}{\omega_{x}} + \frac{i}{(\omega_{x})^{3}} \right)
$$

(285)

(286)

where for convenience we have defined

$$
\theta_{ij} = \delta_{ij} - \hat{x}_{i}\hat{x}_{j},
$$

$$
\phi_{ij} = \delta_{ij} - 3\hat{x}_{i}\hat{x}_{j},
$$

$$
\varphi_{ij} = -\epsilon_{ijk}\hat{x}_{k}.
$$

(287)

(288)

(289)

We remark that due to the causality constraint imposed by the function $\theta(t_{r})$ within the source fields, all results that follow are to be understood as holding for $t_{r} > 0$.

First we calculate the Glauber intensity in the state $|\epsilon^{p}, 0\rangle$ which was used in Sec. V A. Only the first-order field $E_{1}$ contributes, because $I_{G}$ is normal-ordered. The radiation component, which varies as $x^{-2}$ is, within the rotating-wave and Markov approximations, given by

$$
I_{G}^{\text{rad}}(t, x) = \left( \frac{1}{4\pi x} \right)^{2} \sum_{l<p} \omega_{pl}^{3} d_{pl} \cdot \theta \cdot d_{lp}
$$

(290)

in which strict bare-energy conservation is observed. Integrating this expression over a sphere surrounding the dipole gives

$$
\int d\Omega x^{2} I_{G}(t, x) = \frac{1}{2} \sum_{l<p} \omega_{pl}^{3} \Gamma_{pl}
$$

(291)

which is half of the expected radiated energy-flux. The total energy flux is found using the Poynting vector [56, 57, 91, 92]:

$$
S(t, x) := \frac{1}{2} [\mathbf{E}(t, x) \times \mathbf{B}(t, x) - \mathbf{B}(t, x) \times \mathbf{E}(t, x)]
$$

$$
= S_{\text{vac}}(t, x) + S_{\text{real}}(t, x) + S_{\text{virt}}(t, x).
$$

(292)

Note that, as was found in Sec V B 1, the vacuum-source partitioning of a given physical field is gauge-relative and so again the individual components on the right-hand-side of Eq. (292) differ in different gauges, each of which defines the corresponding physical “sources” and “vacuum” differently [29]. We are presently using the multipolar-gauge.

The vacuum component is defined as the part that depends on the vacuum fields alone and so we will focus on the remaining source part. The real and virtual components will be defined below. Using Eqs. (281) and (282) we see that in addition to a normally-ordered combination of first order fields as occurs in the Glauber intensity, there is also an anti-normally ordered contribution from the first order fields, and there are also correlations between the vacuum and second-order fields. The contribution of first order fields to the Poynting vector is
This contribution is transient and rapidly decaying in the sense that, for fixed \( x \), it vanishes both when \( t \gg x \), and when an infinite time-average is taken [56]. It also vanishes if the Markov approximation is performed. However, we saw in Sec. VA that virtual contributions are not necessarily small when averaged over a finite time for sensible ultra-violet cut-offs.

To gain further insight one can calculate the average of the electromagnetic energy-density, which is the sum of electric and magnetic components

\[
\langle \mathbf{E}_{\text{EM}}(t, x) \rangle := \frac{1}{2} \int_0^\infty dt \int d^3x \mathbf{E}(t, x)^2 + \mathbf{B}(t, x)^2
\]

where we have separated-off pure-vacuum contributions into the term \( \mathcal{E}_{\text{vac}}(t, x) \). Again we note that the individual components on the right-hand-side of Eq. (300) differ in different gauges, which each define the corresponding physical “sources” and “vacuum” differently [29]. We are presently using the multipolar-gauge. Both the electric and magnetic source energy-densities \( \mathcal{E}_{\text{E}}(t, x) \) and \( \mathcal{E}_{\text{M}}(t, x) \) respectively, receive contributions from the first order fields as well as from vacuum source-field correlations. Concurrently, both densities can be partitioned into a time-independent component plus a time-dependent component; \( \mathcal{E}_{\text{E}}(t, x) = \mathcal{E}_{\text{E}}^\text{t}(t, x) + \mathcal{E}_{\text{E}}^\text{r}(t, x) \), \( X = E, M \). The time-dependent parts are again purely virtual, but in contrast to the Poynting vector, the time-independent parts also have a virtual component. The time-independent electric energy-density is [56, 57]

\[
\langle \mathcal{E}_{\text{E}}^\text{t}(t, x) \rangle = \frac{1}{16\pi^2} \sum_{l < p} d_{pl} d_{pl}^* \int \omega_{pl}^2 f_{ij}(\omega_{pl} e^{ix}) f_{ij}(\omega_{pl} e^{-ix})\]

while the time-dependent component is

\[
\langle \mathcal{E}_{\text{E}}^\text{r}(t, x) \rangle = \frac{i}{4(2\pi)^3} \int_0^\infty d\omega \omega^3 \times \text{Re} \{ A_p (t, x, \omega) e^{ix} \} + \text{Im} \{ C_p (t, x, \omega) e^{-ix} \} + \text{c.c.}
\]

The time-independent component itself has two distinct parts. For an excited state \( p > 0 \) the first term in Eq. (301) dominates in the far-field, \( x \gg 1/\omega_{pl} \), and corresponds to real photon emission;

\[
\langle \mathcal{E}_{\text{E}}^\text{t}(t, x) \rangle = \frac{1}{16\pi^2} \sum_{l < p} \omega_{pl}^6 \left[ d_{pl} \cdot \theta \cdot d_{pl} \left( \frac{1}{(\omega_{pl} x)^2} - \frac{2}{(\omega_{pl} x)^4} \right) + d_{pl} \cdot \phi \cdot d_{pl} \left( \frac{1}{(\omega_{pl} x)^4} + \frac{1}{(\omega_{pl} x)^6} \right) \right]
\]
In contrast, for a ground state bare dipole, \( p = 0 \), the first term in Eq. (301) vanishes, so only the second term remains. In the near-field \( x \ll 1/\omega_0 \) this term is

\[
\langle \delta_E^1(x) \rangle_0 = \frac{1}{32\pi^2 \omega^6} \sum_l \mathbf{d}_{il0} \cdot \phi^2 \cdot \mathbf{d}_{0l}, \quad \omega_0 x \ll 1.
\]

(304)

which is the electrostatic energy of the dipole. We are now in a position to understand how the the vacuum and source components of the electric energy density would be different if we had instead assumed a Coulomb-gauge dipole prepared in the state \( |e^p,0 \rangle \). In the Coulomb-gauge the electrostatic field is included within the definition of the dipole. Thus, the electric energy-density for \( t_r > 0 \) would be identical to that above whereas for \( t_r < 0 \), \( \delta_E(t,x) \) would have been found to coincide with that in Eq. (304) [29]. Since the multipolar-gauge and Coulomb-gauge vacuum densities also differ by the same amount the sum \( \epsilon_{\text{vac}} + \epsilon_E \) is unique and the same in both gauges. This is consistent with the results of Sec V B1 whereby the vacuum-source partitioning of the electric field itself differs between the Coulomb and multipolar-gauges in precisely this way [Eq. (272)].

Finally we may consider the far-field limit of the first term of Eq. (301) for \( p = 0 \), which is

\[
\langle \delta_E^1(x) \rangle_0 = \frac{1}{64\pi^3} \sum_{l \neq 0} \mathbf{d}_{0l} \cdot \omega_0 (13\delta_{ij} - 7\hat{x}_i \hat{x}_j), \quad \omega_0 x \gg 1.
\]

(305)

possessing the characteristic (Casimir-Polder) \( x^{-7} \) decay. Eqs. (304) and (305) respectively give the near and far-field limits of the virtual part of the time-independent part of the electric energy-density’s multipolar-gauge source-component. Similarly to the above, for the magnetic energy-density we find

\[
\langle \delta_M^1(x) \rangle_0 = \frac{1}{16\pi^2} \sum_{l \neq 0} \mathbf{d}_{0l} \cdot \phi^2 \cdot \mathbf{d}_{0l} g_{ij}(\omega_{00}) g_{ij}(\omega_{00})
\]

\[+ \frac{1}{16\pi^3} \sum_{l} \omega_{pl} \phi_{pl}^2 \int_0^\infty d\omega \omega^3 \]

\[\times \int_0^\infty ^{1} \cos q x \int_0^\infty d\omega \omega^3 \]

\[\times \text{Re}(g_{q}(\omega x) e^{i\omega x}) e^{i\omega x} + \text{c.c.}
\]

and

\[
\langle \delta_M^1(t,x) \rangle = -\frac{i}{4(2\pi)^2} \int_0^\infty d\omega \omega^3
\]

\[\times \text{Re}(g_{q}(\omega x) e^{i\omega x}) e^{i\omega x} + \text{c.c.}
\]

(306)

(307)

The time-independent part again possesses a non-vanishing real-photon part for \( p > 0 \) which dominates in the far-field via \( x^{-2} \) decay, and which vanishes for \( p = 0 \). For \( p = 0 \), the remaining time-independent part exhibits different behaviour in the near and far zone limits similar to the electric energy-density. The near-field limit varies as \( x^{-5} \) rather than \( x^{-6} \), while the far-field limit again decays as \( x^{-7} \). Note that unlike the electric field the vacuum-source partitioning of the magnetic-field is not gauge-relative so the above results for the magnetic energy density are identical in every gauge [29].

The only components not yet discussed are the time-dependent components given by Eqs. (302) and (307). These parts are purely virtual and for \( x \neq 0 \), they comprise the only non-trivial contributions within the local continuity equation for energy. Poynting’s theorem reads:

\[
\frac{d}{dt} \langle \delta_{EM}(t,x) + \delta_d(t,x) \rangle = -\nabla \cdot \langle S(t,x) \rangle
\]

(308)

where \( \delta_d(t,x) \) is the energy density of the bare dipole localised at \( 0 \). For \( x \neq 0 \), this becomes

\[
\frac{d}{dt} \langle \delta_{EM}(t,x) \rangle = -\nabla \cdot \langle S(t,x) \rangle.
\]

(309)

It is noteworthy that the vacuum, real and virtual components of \( S \) separately satisfy local energy conservation as can be directly verified. For the vacuum parts, which are space and time-independent this is immediate. For the time-independent energy-density such that \( d\langle \epsilon_{EM}(t,x) \rangle /dt \equiv 0 \) the corresponding Poynting vector is \( \langle S_{\text{real}}(t,x) \rangle \), which is such that \( \nabla \cdot \langle S_{\text{real}}(t,x) \rangle = 0 \) for \( x \neq 0 \). Therefore, Eq. (309) is also trivially satisfied for the real part of \( S \). The integral of the divergence of the real Poynting vector over a sphere \( \mathcal{S} \) containing the dipole has already been calculated and is given by Eq. (296). Finally, it can be verified using Eqs. (302), (307) and (294) that

\[
\frac{d}{dt} \langle \delta_{EM}(t,x) + \delta_d(t,x) \rangle = -\nabla \cdot \langle S(t,x) \rangle.
\]

(310)

Virtual contributions violate bare-energy conservation by definition whereas global energy conservation is fundamental and is automatically satisfied; \( [H,H] \equiv 0 \). The stronger condition of local energy conservation, namely Eq. (308), is also fundamental, yet its explicit verification is more involved. The calculation above shows that virtual processes do satisfy this fundamental requirement and in this sense they are not unphysical, indicating again that the term virtual is a misnomer.

For simplicity we now restrict our attention to the lowest two-dipole levels with energy difference \( \omega_m \), and calculate the variations in the time-dependent part of the energy-density on the surface of the sphere with radius \( x < t \) surrounding the bare dipole in its ground state. This is found to be

\[
\hat{u}(t,x) := \frac{2\pi}{\omega_m^3} \int d\Omega \frac{d}{dt} \langle \epsilon_{EM}(t,x) \rangle
\]

\[= 8\theta(t_r) \omega_m x q_r q_x \left[ 2q_x \cos q_r + (q_x^2 - 2) \sin q_r \right]
\]

(311)

where we have chosen a spacetime-independent normalisation \( \omega_m^3 \) to obtain a dimensionless measure, and
perturbation theory as
\begin{align}
|E^p_0\rangle &= T |\epsilon^p, 0\rangle = (1 + T_1 + T_2) |\epsilon^p, 0\rangle, \\
T_1 |\epsilon^n, 0\rangle &= \sum_{i\neq p, k\lambda} |\epsilon^i, k\lambda\rangle \frac{|\langle \epsilon^i, k\lambda | V^1 |\epsilon^p, 0\rangle|^2}{\omega + \omega_{ip}}, \\
T_2 |\epsilon^p, 0\rangle &= \sum_{i,j\neq p, k\lambda, k'\lambda'} |\epsilon^i, k\lambda, k'\lambda'\rangle \\
&\quad \times \langle \epsilon^j, k\lambda, k'\lambda' | V^1 |\epsilon^i, k\lambda \rangle \langle \epsilon^j, k\lambda | V^1 |\epsilon^i, k\lambda, k'\lambda'\rangle \\
&\quad \times (\omega + \omega_{jp})(\omega + \omega' + \omega_{ip})
\end{align}

The average Poynting vector in the state $|E^p_0\rangle$ is found to be \cite{57}
\begin{equation}
\langle E^p_0 | S(t, x) | E^p_0 \rangle = \langle S^\text{re}|(t, x) \rangle
\end{equation}
where the right-hand-side is defined as in Eq. (295). This vanishes for $p = 0$ showing that there can be no energy loss in the ground state \cite{57}. On the other hand the electric energy-density in the vicinity of the dipole does not vanish for the ground state and is found to be \cite{57}
\begin{equation}
\langle E^p_0 | \delta E | E^p_0 \rangle = \langle \delta E |(x) \rangle|_{p=0}
\end{equation}
\begin{equation}
= \frac{1}{16\pi^3} \sum_l \omega_{0l} d_{0l} d_{l0} \int_0^\infty du \frac{u^2 e^{-2ux}}{u^2 + \omega_{0l}^2} f_{ij}(iux) f_{ij}(iux)
\end{equation}
where $\langle \delta E |(x) \rangle$ is defined in Eq. (301). Thus, the differences between the ground state predictions found using $|E^0_0\rangle$ and those found using the bare ground state $|\epsilon^0, 0\rangle$ are the time-dependent components $\langle S^{\text{virt}} \rangle$ and $\langle \delta E^t \rangle$.

If the system is prepared in the state $|\epsilon^0, 0\rangle$ in the multipolar-gauge, then $\langle \delta E^t \rangle$ represents the only part of the full average $\langle \delta E^t \rangle$ that is not typically neglected, that is, the purely virtual part $\langle \delta E^t \rangle$ is often ignored \cite{56}. Within this approximation we have $\langle \delta E^t \rangle = \langle \delta E^t |(x) \rangle|_{p=0}$

\begin{equation}
\langle \delta E^t \rangle|_{p=0} = \langle \delta E^t |(x) \rangle - \langle \delta E^t \rangle|_{p=0}
\end{equation}
consistent with the results of Sec. IV B 2 in which the dipole’s stationary state was found within the conventional weak-coupling approximations to be the bare ground state.

Let us now again consider the example of the harmonic dipole as in Sec. VA. In this case the full ground state is represented by the vacuum $|0, 0\rangle$ of light and matter modes $c$ and $d$ defined relative to the JC-gauge. These modes are specified by Eqs. (252)-(256). In the JC-gauge the canonical momentum $\Pi(x)$ represents the physical observable $O_{JC}(x) = -D_T(x) + P_T(x) - P_{TJC}(x)$ where to order $q^2$
\begin{equation}
P_T(x) - P_{TJC}(x) = \sum_{k\lambda} \frac{\epsilon_{k\lambda}}{u} \frac{\epsilon_{k\lambda} \cdot d}{\omega + \omega_{im}} e^{ikx}.
\end{equation}
The electric field is therefore given for $x \neq 0$ by $E = -\Pi + P_T - P_{TJC}$. Writing $\Pi$ in terms of the modes $c_k$.
we find the average using the vector \( |0_d, 0_c\rangle \) to be
\[
\langle \Pi(\mathbf{x}) \rangle_0 = \sum_{k,j} q^2 \frac{(e_k \cdot e_j)}{2m\omega_m \nu^2} \frac{\omega_m \omega_k \omega_j e^{i(k+j) \cdot \mathbf{x}}}{(\omega_k + \omega_j)(\omega_m + \omega_j)}
\]
(318)

where we have labelled the modes using a single index as in Sec. V.A. Using Eq. (317), one can show that, as required, \( \langle \mathcal{E}_E \rangle_0 = \langle \Pi^2 + |P_T - P_TJC|^2 \rangle_0 / 2 \) coincides with the electric energy-density in Eq. (316) when assuming a harmonic dipole. We see therefore that the average \( \langle \mathcal{E}_{EM} \rangle \) is found to coincide with \( \langle \mathcal{E}_{EM}^{K} \rangle = \langle \mathcal{E}_{EM}^{K} \rangle_0 \), without neglecting (as a weak-coupling or Markov approximation) any time-dependent component \( \langle \mathcal{E}_{EM}^{T} \rangle \), provided that the subsystems are defined relative to the JC-gauge. The prepared state then coincides with the true ground state.

### 3. Discussion

Above we have compared the same physical observable, namely the electromagnetic (EM) energy-density, while assuming different initial physical states. These different states are ones of well-defined energy of different physical subsystems. When choosing the multipolar-gauge, the vector \( |\epsilon^0, 0\rangle \) specifies a localised “bare” dipole in its own lowest energy state and with no accompanying photons. In this case the EM energy-density possesses a virtual time-dependent component \( \langle \mathcal{E}_{EM}^{V} \rangle \). The same vector \( |\epsilon^0, 0\rangle \) in the Coulomb-gauge specifies an electrostatically dressed dipole with no accompanying photons. Thus, the same EM energy-density is obtained as in the multipolar-gauge, with the exception that for \( \tau < 0 \) we obtain a non-vanishing electrostatic energy-density given by Eq. (304).

In the case of a harmonic dipole, the vector \( |0_d, 0_c\rangle \) specifies a state of well-defined energy of the subsystems defined relative to the JC-gauge and this coincides with the ground state. In this case the EM energy-density is again the same but possesses no time-dependent virtual component. This is consistent with an interpretation of the JC-gauge subsystems as having subsumed the virtual ground state quanta that exist in conventional gauges.

The most relevant physical predictions will depend on which of these physical states is closest to that which has been prepared in the experiment considered. This, in turn, will depend on the extent to which the purely virtual field that results in the energy-density \( \langle \mathcal{E}_{EM}^{V} \rangle \), is separate from the addressable dipole. The transient and highly localised nature of this field suggest that it should be considered part of the dipole on the accessible time and length scales. However, this may depend on the available preparation and measurement procedures. Similarly, in stronger-coupling regimes, whether or not the ground state is entangled and contains a large number of photons depends on the gauge-relative to which the subsystems are defined, i.e., on the relative extent to which the virtual bound-field is taken as separate from the physical (measurable) dipole.

### D. Cavity QED beyond weak-coupling approximations

We now turn our attention to understanding photonic fields confined to a cavity where weak-coupling theory is generally inapplicable and subsystem gauge-relativity is expected to be important.

#### 1. Intra-cavity fields

We first consider a simple analysis of intra-cavity fields produced by a dipole at the cavity centre. This closely mirrors the above analysis in Sec. V.C.2 for free space. An early step towards evaluating the Glauber intensity within a cavity in the ultrastrong-coupling regime has been given in [63]. Therein emphasis was placed upon the need for a multi-mode theory in accommodating the requisite spatio-temporal structure to elicit signal propagation. We will consider a similar analysis in an arbitrary-gauge.

We model the cavity as a one-dimensional field in the \( z \)-direction with periodic boundary conditions at \( x = \pm L/2 \) where \( L \) is the cavity length. The allowed wavenumbers are \( k = 2\pi n / L, \ n \in \mathbb{Z} \). The canonical fields are assumed to point in the \( z \)-direction and have bosonic mode expansions
\[
A(t, x) = \sum_k \frac{1}{\sqrt{2\omega_k v}} \left[ a_k^\dagger(t) e^{-ikx} + a_k(t) e^{ikx} \right],
\]
(319)
\[
\Pi(t, x) = i \sum_k \frac{\omega_k}{2v} \left[ a_k^\dagger(t) e^{-ikx} - a_k(t) e^{ikx} \right]
\]
(320)

where \( v \) is the cavity volume. The cross-sectional area is therefore \( v/L \). As usual, we have \( |a_k, a_k^\dagger| = \delta_{kk'} \) and \( \omega_k = |k| \). To be consistent with the assumption the expressions for \( \mathbf{A_T} \) and \( \Pi \) the transverse polarisation \( \mathbf{P}_{Ta} \) is also assumed to point in the \( z \)-direction. If we assume further that the dipole within the cavity is anharmonic we may perform a two-level truncation. The final \( \alpha \)-gauge polarisation is therefore defined as
\[
\mathbf{P}_{T\alpha}(t, x) = \sum_k \frac{d}{v} \sigma^\alpha(t) \alpha \cos[kx]
\]
(321)

where \( d = \hat{z} \cdot \mathbf{d} \) is the two-level transition dipole moment in the \( z \)-direction. We note also that since \( \mathbf{P}_{T\alpha} \) commutes with gauge-fixing transformations, Eq. (321) is independent of the gauge within which truncation is performed. To obtain the Hamiltonian, we assume truncation within the multipolar-gauge giving the multipolar-gauge multi-
mode QRM

\[ H_t^2 = \tilde{\omega}_m \sigma^+ \sigma^- + \sum_k \omega_k \left( a_k^\dagger a_k + \frac{1}{2} \right) + i \sum_k g_k (a_k^\dagger - a_k) \sigma^x \]  
(322)

where \( g_k = d \sqrt{\omega_k/2v} \) and we have absorbed the multipolar-gauge polarisation self-energy term into a renormalisation of the two-level transition frequency denoted \( \tilde{\omega}_m \).

In Ref. [63] (see also [94]) it was demonstrated via comparison with numerical results utilising matrix product states that for sufficiently large coupling strengths and numbers of modes the two-level system frequency \( \tilde{\omega}_m \) may be neglected in Eq. (322) resulting in an independent-boson model;

\[ H_t^2 \approx \sum_k \omega_k \left( a_k^\dagger a_k + \frac{1}{2} \right) + i \sum_k g_k (a_k^\dagger - a_k) \sigma^x. \]
(323)

Since \( \sigma^x \) is now a symmetry, the Hamiltonian is easily diagonalised using a polaron transformation

\[ T_{10} = \exp \left[ i \sum_k g_k \left( a_k^\dagger + a_k \right) \sigma^x \right]. \]
(324)

Notice that this is the same type of transformation as was encountered in Sec. III. Although it is not a gauge transformation, we noted in Sec. III E that when acting on the canonical momentum \( \Pi \) this transformation does have the same effect as the projected PZW gauge-fixing transformation \( PR_{10} \) where \( R_{10} \) transforms between the multipolar and Coulomb gauges.

Note also that although two-level truncation has been performed in the multipolar-gauge, we are free to consider the canonical field \( \Pi \) defined relative to an arbitrary gauge \( \alpha \). The physical observable represented by the momentum \( \Pi \) in the gauge \( \alpha \) will be denoted \( O_\alpha \). The notation \( \Pi \) will be reserved for the multipolar-gauge canonical momentum \(-D_T\), therefore \( O_\alpha = \Pi + P_{T1} - P_{Ta} \). The dynamics of the observables \( O_\alpha \) closely mirror those found for free space in Sec. V B 1. Using Eqs. (323) we obtain

\[ a_k(t) = a_k e^{-i \omega_k t} + g_k \int_0^t ds e^{-i \omega_k(t-s)} \sigma^x(s) \]
\[ \equiv a_{k,vac}(t) + a_{k,s}(t). \]
(325)

We note that the above vacuum-source partitioning is that given by the multipolar-gauge. This is the most convenient partitioning if we wish to determine averages when assuming an initial bare state in the multipolar-gauge, which corresponds to assuming a well-defined state of energy of a fully localised dipole. The operator \( \sigma^x(s) = \sigma^x(0) = \sigma^x \) is time-independent because the two-level dipole energy has been neglected. As a result the temporal integral in Eq. (325) can be evaluated immediately, to give

\[ O_\alpha(t,x) = \Pi_{vac}(t,x) + O_{\alpha,s}(t,x), \]
(326)
\[ \Pi_{vac}(t,x) := i \sum_k \sqrt{\frac{\omega_k}{2v}} \left[ a_k^\dagger e^{-i k x + i \omega_k t} - a_k e^{i k x - i \omega_k t} \right], \]
(327)
\[ O_{\alpha,s}(t,x) := \sum_k \frac{d}{v} \sigma^x \left( \cos[k \omega - \omega_k t] - \alpha \cos[k \omega] \right) \]
\[ \equiv \Pi_s(t,x) + P_{T1}(t,x) - P_{Ta}(t,x) \]
(328)

where since \( \sigma^x \) is stationary, so too is the electrostatic field \( P_{Ta}(t,x) = P_{Ta}(0,x) \) defined in Eq. (321). Negative frequency fields are defined as

\[ \Pi_s^{(-)}(t,x) := i \sum_k \sqrt{\frac{\omega_k}{2v}} a_k^\dagger e^{-i k x + i \omega_k t} \]
(329)
\[ \Pi^{(-)}(t,x) := i \sum_k \sqrt{\frac{\omega_k}{2v}} a_k^\dagger(t) e^{-i k x} \]
\[ = \sum_{k>0} \frac{d}{v} \sigma^x \left( e^{i \omega_k t} - 1 \right) \cos[k \omega], \]
(330)
\[ P_{Ta}^{(-)} := \sum_k \frac{d}{2v} \sigma^x \alpha e^{-i k x} = \frac{1}{2} P_{Ta}, \]
(331)

where the integer \( N \) sets the total number of modes retained within the model. More generally, for \( O_\alpha \) this gives

\[ O_\alpha^{(-)}(t,x) = \Pi_{vac}^{(-)}(t,x) + O_{\alpha,s}^{(-)}(t,x), \]
(332)
\[ O_{\alpha,s}^{(-)}(t,x) = \Pi_s^{(-)}(t,x) + P_{T1}^{(-)}(t,x) - P_{Ta}^{(-)}(t,x) \]
\[ = \frac{d}{2v} \sigma^x \left( 1 - \alpha \right) + \sum_{k>0} \frac{d}{v} \sigma^x \left( e^{i \omega_k t} - \alpha \right) \cos[k \omega]. \]
(333)

Positive frequency components are obtained by hermitian conjugation. By construction these expressions yield \( O_\alpha = O_\alpha^{(-)} + O_\alpha^{(+)} \) for any \( \alpha \). Choosing \( \alpha = 1 \) gives the particular case \( O_1 = \Pi = -D_T = -E_T - P_{T1} \).

It is now possible to evaluate the average of arbitrary functions of \( O_\alpha, O_\alpha^{(-)} \) and \( O_\alpha^{(+)} \) using any initial state. We use both the initial multipolar bare state \( |\epsilon^1, 0\rangle \) and the ground state, which is represented by the vector \( |\epsilon^0, 0\rangle \) in the polaron frame. Since we have neglected the dipole energy and since the polaron transformation coincides with the projected PZW transformation when acting on \( \Pi_s \), for the purpose of finding the dynamics of \( O_\alpha \) the polaron-frame is nothing but the Coulomb-gauge. Specifically, we have

\[ T_{10} \Pi T_{10}^\dagger = \Pi - P_{T1}, \]
(334)
\[ T_{10} O_\alpha T_{10}^\dagger = \Pi - P_{Ta}. \]
(335)
cur without the simplifications made. In general, these
calculations approximately purely electrostatic, as shown by
Eqt. (304). We emphasise that the coincidence of the
gauge; m

FIG. 9: The averages \( \langle D^{-}_{T}(t,x)D^{+}_{T}(t,x) \rangle \) (a) and
(\( E^{-}_{T}(t,x)E^{+}_{T}(t,x) \rangle \) (b) are plotted with space and time,
showing the presence and absence of a bound-field around
the multipolar and Coulomb-gauge dipoles respectively. Es-
entially the same propagating field is obtained in both cases.
We have assumed \( N = 50 \) and normalised both densities via
the maximum value attained when the propagating field is
coincident with the dipole; \( (t,x) = (nL,0), \ n \in \mathbb{Z} \).

Since the operator \( T_{10}^{\dagger}T_{10}^{\dagger} \) represents the observable
\(-D_{T} \) in the polaron frame, the operator \( T \) represents the
observable \(-D_{T} + P_{T} \), as in the Coulomb-gauge. In this gauge the electrostatic field is absorbed into
the definition of the dipole. Further still, within the approxima-
tions made the Coulomb-gauge coincides with the JC-
gauge; \( \alpha_{JC} = \tilde{\omega}_{m}/(\tilde{\omega}_{m} + \omega_{k}) \approx 0 \). Thus, the very simple
treatment in which the free dipole Hamiltonian has been
neglected, is unable to distinguish between electrostatic and
virtual-photon bound-fields. We saw in Sec. V C 2 that this distinction is also obscured when considering
the near-field limit of the ground-state energy-density in
free space whereby the total electric energy-density be-
comes approximately purely electrostatic, as shown by
Eqt. (304). We emphasise that the coincidence of the
Coulomb-gauge, the JC-gauge, and the polaron-frame
for calculating averages of functions of \( \Pi \) does not oc-
cur without the simplifications made. In general, these
representations are distinct.

We now calculate various quadratic energy-densities as
in Sec. V C 2. For the initial state \( |\epsilon_{1},0\rangle \) we obtain
\[
\langle O_{\alpha}(t,x)^{2} \rangle - E_{vac} = \left[ \sum_{k} \frac{d}{v} \cos[kx - \omega_{k}t] - \alpha \cos[kx] \right]^{2} \tag{336}
\]
\[
\langle O_{\alpha}^{-}(t,x)O_{\alpha}^{(+)}(t,x) \rangle = \frac{d}{2v} (1 - \alpha) + \sum_{k > 0} \frac{d}{v} (e^{\omega_{k}t} - \alpha) \cos[kx]^{2} \tag{337}
\]
where \( E_{vac} = \sum_{k} \omega_{k}/(2v) \) is an energy-density of the vacuum. For \( \alpha = 1 \) (multipolar-gauge), Eq. (337) reduces
to the result obtained in Ref. [63]. The ground-state
averages of the same operators as above are obtained using
the polaron frame and are found to be
\[
\langle O_{\alpha}(t,x)^{2} \rangle_{G} - E_{vac} = \langle P_{T_{\alpha}}(t,x)^{2} \rangle_{G}, \tag{338}
\]
\[
\langle O_{\alpha}^{-}(t,x)O_{\alpha}^{(+)}(t,x) \rangle_{G} = \frac{1}{4} \langle P_{T_{\alpha}}(t,x)^{2} \rangle_{G} \tag{339}
\]
where
\[
\langle P_{T_{\alpha}}(t,x)^{2} \rangle_{G} = \left[ \sum_{k \neq 0} \frac{d}{v} \alpha \cos[kx] \right]^{2} \tag{340}
\]
This confirms that, within the approximations made, the
bound-field tied to the \( \alpha \)-gauge dipole is nothing but the electrostatic field \( P_{T_{\alpha}} \). In the Coulomb-gauge
this field is fully included within the definition of the dipole, so \( \langle O_{0}(t,x)^{2} \rangle_{G} - E_{vac} = 0 \). Fig. 9 shows
\( \langle O_{\alpha}^{-}(t,x)O_{\alpha}^{(+)}(t,x) \rangle \) given in Eq. (337) for the Coulomb and
multipolar-gauges \( \alpha = 0 \) and \( \alpha = 1 \) respectively.
It can be seen clearly that all gauges possess essentially
the same propagating fields. In contrast the ground-state
bound-field energy has weight \( \alpha^{2} \) within the gauge \( \alpha \) and
is evidently highly localised at the position of the dipole
within the one-dimensional model employed.

Ref. [63] proposes that the initial multipolar bare-state
\( |\epsilon_{1},0\rangle \) could be prepared by controlling the interaction.
However, given the level of localisation of the bound field,
itis far from clear that the latter could ever be separated
from the dipole allowing the corresponding interaction to
be controlled. A possible exception may be to move the
dipole in and out of the cavity very quickly. As already
described in Sec. IV C in this case the relevant gauge for
modelling the interaction using a time-dependent cou-
pling will depend strongly on the microscopic details of
the system.

We remark that the treatment of this section is highly
idealised. The cavity is taken as one-dimensional, the
two-level truncation has also been made, and the dipole
moment dynamics have been taken as approximately sta-
nionary. The extension of these results using more real-
istic treatments warrants further investigation, including
a more physical model for the cavity and a more sophis-
ticated method of solution, for example, via a variational
polaron ansatz [95].
Evidently, the physical nature of the internal cavity field depends strongly on the gauge relative to which it is defined. As we have emphasised, gauge-ambiguities arise because it is not always clear which subsystems should be considered operationally addressable. The interaction between the system of interest and apparatus used in preparation and measurement must be defined relative to a choice of gauge. Next we discuss models for the weak measurement of intra-cavity subsystems.

2. Weak-measurements

The explicit modelling of measurements of light and matter subsystems via a pointer system was considered in the form of simple gedanken experiments by Compagno et al. [18–22]. Such models indicate how measurement procedures might be related to subsystem dressing. To review the weak measurement concept we consider first a bare two-level system coupled to a “macroscopic” pointer with large mass \( M \) and position and momentum \( r \) and \( p \) with \([r, p] = i\) [96]. The position of the pointer is assumed to provide information about the energy of the two-level system. Hence, the Hamiltonian is taken to be

\[
H = \omega_m \sigma^z + \frac{p^2}{2M} + \eta(t)p\sigma^z
\]  

(341)

where \( \sigma^z = [\sigma^+, \sigma^-]/2 \) and where \( \eta(t) \) is a dimensionless system-pointer coupling envelope determining the speed and duration of the interaction, which is assumed to vanish at the initial and final times. We take an initially uncorrelated state of the system and pointer with a sharp Gaussian distribution of pointer positions, with standard deviation \( \sigma \) and centre at \( r = 0 \);

\[
|\psi(0)\rangle = \frac{1}{(2\pi\sigma^2)^{\frac{1}{4}}} \int dr \, e^{-r^2/(4\sigma^2)} \sum_i c_i |e^i, r\rangle.
\]  

(342)

Compagno et al. assume an instantaneous switching function [22]

\[
\eta(t) = \frac{r}{t_P} [\theta(t) - \theta(t - t_P)]
\]  

(343)

where \( t_P \) is the measurement duration after which the pointer’s position is observed. The parameter \( r \) has the dimensions of \( r \). The evolution operator is

\[
U(t) = e^{-iHt} e^{-i\sigma^z p}
\]  

(344)

where \( h = \frac{p^2}{2M} + \omega_m \sigma^z \) generates free evolution. The state at time \( t \) in the interaction picture with respect to \( h \) is

\[
|\psi(t)\rangle = \frac{1}{(2\pi\sigma^2)^{\frac{1}{4}}} \int dr \, e^{-r^2/(4\sigma^2)}
\times \left( c_0 |e^0, r - t/2\rangle + c_1 |e^1, r + t/2\rangle \right)
\]  

(345)

The diagonal matrix elements in the position basis of the corresponding reduced pointer state are therefore

\[
P_t(r) := \langle r | \rho(t) | r \rangle = \frac{1}{\sqrt{2\pi\sigma}} \left( p_0 e^{-(r+t/2)^2/(2\sigma^2)} + p_1 e^{-(r-t/2)^2/(2\sigma^2)} \right)
\]  

(346)

where \( p_1 = |c_1|^2 \) and \( p_0 = 1 - p_1 = |c_0|^2 \) are the excited and ground state probabilities. Thus, the system pointer coupling splits the initial single Gaussian peak into two Gaussian peaks at \( \pm t/2 \) with relative heights that give the probabilities to find the two-level system excited or not excited. In this sense, the pointer measures the energetic state of the two-level system.

Ignoring the free evolution, the average \( \langle r(t) \rangle \) and variance \( \langle \langle r(t) \rangle \rangle := \langle r(t)^2 \rangle - \langle r(t) \rangle^2 \) of the pointer position at time \( t \) are easily found using Eq. (345) to be

\[
\langle r(t) \rangle = r \left( p_1 - \frac{1}{2} \right) = r \sigma^z_0,
\]  

(347)

\[
\langle \langle r(t) \rangle \rangle = r^2 p_1 (1 - p_1) + \sigma^2 = r^2 \left( \frac{1}{4} - \langle \sigma^z \rangle_0^2 \right) + \sigma^2
\]  

(348)

where on the right-hand-sides \( \langle \rangle_0 \) denotes averaging in the initial state and \( \sigma^z \equiv \sigma^z(0) \). We may assume that the initial Gaussian state is sharp with vanishingly small variance, \( \sigma \to 0 \), such that the final term \( \sigma^2 \) in Eq. (348) can be ignored. The average pointer position and variance are sufficient to deduce the important features of the distribution of pointer positions whose diagonal matrix elements are \( P_t(r) \). Specifically, when \( p_1 = 0 \) (ground state dipole) there is a peak in the distribution of pointer positions at \( \langle r(t) \rangle = -r/2 \) and there are no other peaks, consistent with \( \langle \langle r(t) \rangle \rangle = 0 \). Similarly, when \( p_1 = 1 \) (excited dipole) there is a peak at \( \langle r(t) \rangle = +r/2 \) and there are again no other peaks: \( \langle \langle r(t) \rangle \rangle = 0 \). For \( p_1 = 1/2 \) we have \( \langle r(t) \rangle = 0 \) and \( \langle \langle r(t) \rangle \rangle = r^2/4 \), corresponding to symmetric peaks at \( \pm r/2 \), which indicate equal probabilities that the detector will register the dipole in either of its two states.

Compagno et al. considered the same dipole-pointer interaction and the same initial pointer state in the case of a two-level dipole coupled to a single radiation-mode with polarisation \( e \) and frequency \( \omega \) in volume \( v \), starting in the ground state of the dipole-mode system [22]. More generally, we can consider light and matter subsystems defined relative to an arbitrary-gauge specified by \( \alpha(\omega) \). To order \( q^2 \) we obtain

\[
\langle r(t) \rangle = r \, \langle \sigma^z \rangle,
\]  

(349)

\[
\langle \langle r(t) \rangle \rangle = r^2 \left( \frac{1}{4} - \langle \sigma^z \rangle^2 \right) \sin^2 \left[ \frac{1}{2} (\omega_m + \omega) t_P \right],
\]  

(350)

where \( \sin x := \sin(x)/x \) and

\[
\langle \sigma^z \rangle \equiv \langle \sigma^z(0) \rangle = -\frac{1}{2} + \frac{|e \cdot d|^2 \omega_m u^+ + \omega^2}{2v} \frac{u_m + \omega}{(\omega_m + \omega)^2}
\]  

(351)
in which $u^+(\omega)$ is the coefficient defined in Eq. (262) of counter-rotating terms within the bilinear $\alpha(\omega)$-gauge interaction Hamiltonian.

We see that the choice of gauge determines the physical model for the pointer, which is implicitly assumed to couple to the dipole quantum subsystem defined relative to the $\alpha(\omega)$-gauge. In particular, the gauge choice determines the extent to which the pointer is defined as being able to register ground state virtual photons, which arise from counter-rotating terms. In the JC-gauge the ground state of the dipole-mode system simply comprises a ground state dipole JC and no photonsJC, such that $u^+(\omega) \equiv 0$ and therefore $\langle r(t) \rangle = -t/2$ and $\langle \langle r(t) \rangle \rangle = 0$ for all times. These are identical to the previous results for an uncoupled ground-state dipole [the $p_1 = 0$ cases of Eqs. (347) and (348)]. Thus, the relative strength of the counter-rotating terms within the interaction, as specified by $u^+(\omega)$, determines the relative deviation from the case of a ground state dipoleJC, which looks to the pointer exactly the same as an uncoupled ground state dipole. In this sense $\alpha(\omega)$ directly controls the degree of virtual dressing explicitly registered by the pointer.

For $u^+(\omega) \neq 0$ the pointer position's variance is time-dependent due to the addition of the sinc-function, which represents the (bare) energy-time uncertainty relation as encountered in Sec. V A. This means that as well as the dipole's definition, the dressing registered by the pointer also depends on the measurement duration compared with bare cycle times. For short measurements compared with a bare cycle, $t_P(\omega_m + \omega) \ll 1$, the average and variance again reduce to the uncoupled dipole result, such that the dipole appears to the pointer as being the same as an uncoupled ground state dipole. For long measurements $t_P(\omega_m + \omega) \gg 1$ the variance vanishes, indicating a single peak in the distribution of pointer positions, but not one located at $-t/2$ as for an uncoupled dipole, instead the peak's position is determined by Eqs. (349) and (351). This will be the same as the uncoupled dipole case only for gauges sufficiently close to the JC-gauge. In this way, the extent to which the dipole appears to the pointer as being the same as an uncoupled bare dipole is controlled by the balance between $u^+(\omega)$ and the measurement duration $t_P$. For a given $u^+(\omega)$ longer measurements result in increasing deviation from the uncoupled dipole case, while for fixed $t_P$ a larger $u^+(\omega)$ similarly results in increased deviation.

We can extend these results to the multi-mode case [22]. Again taking the ground state of the dipole-field system we obtain in the mode-continuum limit and to order $q^2$

$$\langle r(t) \rangle = \frac{r}{2} \left( -1 + \frac{\Gamma}{\pi} \int_0^\infty d\omega \left[ \frac{u^+(\omega)}{\omega_m(\omega_m + \omega)} \right]^2 \right), \quad (352)$$

$$\langle \langle r(t) \rangle \rangle = \frac{r^2 \Gamma}{2\pi} \int_0^\infty d\omega \left[ \frac{u^+(\omega)}{\omega_m(\omega_m + \omega)} \right]^2 \text{sinc} \left[ \frac{1}{2}(\omega_m + \omega) t_P \right]. \quad (353)$$

Again, in the JC-gauge the result is identical to a ground state uncoupled dipole, because again the ground state of the dipole-field system simply comprises a ground state dipoleJC and no photonsJC, such that $u^+(\omega) \equiv 0$. On the other hand, in the multipolar-gauge we have $u^+(\omega)^2 = \omega/\omega_m$ while in the Coulomb-gauge $u^+(\omega)^2 = \omega_m/\omega$. For fixed $\omega_m$, high-frequency modes are seen to contribute less and the low frequency modes more in the Coulomb-gauge as compared with the multipolar-gauge. High-frequency multipolar-modes are instead included as explicit electrostatic interactions in the Coulomb-gauge so their contributions already belong to the dipoleJC. Concurrently, for fixed $\omega$ the contribution of the dipole frequency $\omega_m$ is larger within the Coulomb-gauge. The results closely mirror the photodetection probabilities given in Sec. V A. In the Markovian regime the multipolar-gauge average pointer position is quadratically divergent with an ultraviolet cutoff, whereas the corresponding Coulomb-gauge result is logarithmically divergent. The multipolar-gauge pointer position variance is logarithmically divergent whereas the corresponding Coulomb-gauge result is convergent.

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The weak-measurement formalism is general in that it is obviously not restricted to any particular subsystem or observable. It can be used to model the measurement of arbitrary light or matter subsystem observables. However, a generic feature of weak-measurements in QED is that a gauge must be selected relative to which the subsystem that the pointer couples is defined. Each gauge then provides a description of a different physical measurement process. Furthermore, since the system-pointer coupling is by assumption controllable, it is modelled via an explicitly time-dependent coupling, and so the considerations of Sec. IV C apply. Specifically, the assumption that the system-pointer coupling is time-dependent is not a gauge-invariant assumption. Distinct models resulting when this assumptions is made in distinct gauges describe different experimental protocols and will yield different predictions even for the pointer's measurement of the same physical observable. We end by remarking that the extension of the simple framework presented in this section to ultrastrong-coupling regimes and specific experimental contexts warrants further study.

3. **Ground state superradiance**

Here we exemplify the importance of the preceding discussions concerning intra-cavity fields and subsystem gauge-relativity by very briefly reviewing the phenomenon of ground state superradiance, as first predicted in the Dicke model [97–99]. There is now extensive literature on this topic including extended Dicke models [100–104], connections with quantum chaos [105–107], driven and open systems [108–112], and artificial systems [11, 113–123]. The topic has received renewed interest in light of rapid progress in magnonic systems and in controlling correlated electron systems inside cavities [124–129].
Despite this, whether or not a phase transition does indeed occur and its precise nature have remained fundamental open questions. This is due to the existence of so-called “no-go theorems”, which prohibit a superradiant phase and which are proved in the Coulomb-gauge [130]. Further variants of this theorem have been given and have been both refuted and confirmed subsequently [47, 103, 104, 113, 116, 116, 120, 122, 125, 131–139].

Keeling noted that since the radiation modes are distinct in the Coulomb and multipolar gauges, a ground state transition may possess different characterisations and showed that a ferroelectric phase transition occurs within the Coulomb-gauge at the same point in parameter space as the superradiant phase transition of the conventional Dicke model [136]. More recently, the present authors have shown [6] that a unique (gauge-invariant) phase transition can be supported within cavity QED systems, by using the one-parameter $\alpha$-gauge framework. It was shown further that the macroscopic manifestation is gauge-invariant, but that the classification of the phase transition depends on the gauge relative to which the quantum subsystems are defined.

For a cavity containing $N$ dipoles labelled by $\mu = 1, \ldots, N$, with dipole moments $d_\mu$ and fixed positions $R_\mu$, the $\alpha$-dependent canonical momenta are found to be $[6]$ 

$$p_{\mu\alpha} = m \dot{r}_{\mu} - e(1 - \alpha)A(R_\mu),$$

$$\Pi_\alpha(x) = -E_T(x) - p_{T\alpha}(x),$$

The Hamiltonian is the total energy $[6]$

$$H = \sum_{\mu=1}^{N} \frac{1}{2} m \dot{r}_{\mu}^2 + V + V_{\text{dip}} + \frac{1}{2} \int d^3x \left[ E_T(x)^2 + B(x)^2 \right].$$

where the electrostatic energy has been split into an atomic binding energy for each dipole, $V$, and an interdipole electrostatic coupling, $V_{\text{dip}}$ (dipole-dipole interaction). The Hamiltonian expressed in terms of canonical operators and within the EDA is

$$H = \sum_{\mu=1}^{N} \frac{1}{2m} \left[ p_{\mu\alpha} + e(1 - \alpha)A(T(R_\mu)) \right]^2 + V + \frac{\alpha^2}{2} \sum_{\mu=1}^{N} d_{\mu,i}d_{\mu,j}b_{\mu i}^\dagger b_{\mu j} + (1 - \alpha^2)V_{\text{dip}} + \alpha \sum_{\mu=1}^{N} d_{\mu} \cdot \Pi_{T\alpha}(R_\mu) + \frac{1}{2} \int d^3x \left[ \Pi_{T\alpha}(x)^2 + B(x)^2 \right].$$

Assuming that the dipole moments $d = d \cdot e$ point in the direction of the cavity polarisation $e$, the single-mode approximation is performed in such a way as to preserve gauge-invariance (see Secs. II F and II O 2). This eliminates the need to regularise $P_T$ [46], and ensures that the transverse commutation relation for the canonical fields is preserved. The fundamental kinematic relations given by Eqs. (354) and (355) are therefore also preserved. In order to obtain a Dicke Hamiltonian the limit of closely spaced dipoles around the origin, $R_\mu \approx 0$ is taken, and the dipoles are approximated as two-level systems. Collective operators are then introduced;

$$J^i_\alpha = \sum_{\mu=1}^{N} \sigma^i_{\mu\alpha}, i = \pm, z,$$

where $\sigma^\pm_{\mu\alpha}$ are the raising and lowering operators of the $\mu$th two-level dipole and $\sigma^\alpha_{\mu\alpha} = [\sigma^+_{\mu\alpha}, \sigma^-_{\mu\alpha}] / 2$.

We also introduce cavity bosonic operators $c_\alpha$ and $c_\alpha^\dagger$, which incorporate both the bare cavity energy and the $A^\ast$-term in Eq. (357). The resulting arbitrary-gauge Dicke Hamiltonian is

$$H^{\alpha,2} = \omega_m J^+_\alpha + \frac{N}{2} (e_\alpha + e_\alpha^\dagger) + \frac{1}{2} \rho d^2 + \omega_\alpha \left( c^\dagger_\alpha c_\alpha + \frac{1}{2} \right) - \frac{C_\alpha}{N} (J^+_\alpha + J^-_\alpha)^2 - i \frac{g_\alpha}{\sqrt{N}} (J^+_\alpha - J^-_\alpha)(c^\dagger_\alpha + c_\alpha) + i \frac{g_\alpha}{\sqrt{N}} (J^+_\alpha + J^-_\alpha)(c^\dagger_\alpha - c_\alpha),$$

where $\omega_m = e_\alpha - e_\alpha^\dagger$, $\omega_\alpha = \omega^2 + e^2 - (1 - \alpha^2)\rho / m$, $C_\alpha := \rho d^2 - (1 - \alpha^2) / 2$, $g_\alpha := (1 - \alpha)\omega_m d \rho / (2\omega_\alpha)$, and $g_\alpha := \alpha d \rho / (2\omega_\alpha)$, with $d = e \cdot d$. Here $\rho = N/v$ remains finite in the thermodynamic limit $N \to \infty$, $v \to \infty$. Although the non-truncated Hamiltonian $H$ is unique, we now have a continuous infinity of Dicke Hamiltonians $H^{\alpha,2}$ such that $H^{\alpha,2}$ and $H^{\alpha,2}$ are not equal when $\alpha \neq \alpha'$ [4, 7–9]. The breaking of gauge-invariance due to truncation turns out not to be a barrier in eliminating all ambiguities regarding the occurrence and nature of a quantum phase transition.

To take the thermodynamic limit the Holstein-Primakoff map defined by

$$J^i_\alpha = b^\dagger_\alpha b_\alpha - N/2,$$

$$J^0_\alpha = \frac{b^\dagger_\alpha \sqrt{N - b^\dagger_\alpha b_\alpha}},$$

$$J^0_\alpha = (J^0_\alpha)^\dagger,$$

where $[b_\alpha, b^\dagger_\alpha] = 1$, is used [105–107]. The Hamiltonian obtained by substituting these expressions into Eq. (359) is denoted $H^{\alpha,2}$. The thermodynamic-limit is defined by $N \to \infty$ and $v \to \infty$ while $\rho = N/v$ remains finite. In this limit the total Hamiltonian in Eq. (359) is found to support two distinct phases and reads

$$H^{\alpha,2,2}_{\text{th}} = E^i_\alpha f^i_\alpha f^\dagger_\alpha + E_\alpha^\dagger c_\alpha c_\alpha^\dagger + \frac{1}{2} (E^0_\alpha + E^0_\alpha^\dagger) + C^i$$

(363)
where the superscript $i$ is either $i = n$ for normal-phase, or $i = a$ for abnormal-phase. The polariton operators $f^i_\alpha, c^i_\alpha$ are bosonic satisfying $[f^i_\alpha, f^j_\alpha] = 1 = [c^i_\alpha, c^j_\alpha]$ with all other commutators vanishing. The polariton energies $E^{\alpha, i}_{\alpha, \beta}$ and constant $C^i$ are known functions of the couplings and frequencies appearing in the Hamiltonian of Eq. (359). It can be shown that the lower polariton energy $E^n_\alpha$ is real provided that

$$\tau := \frac{\omega_m}{2pd^2} \geq 1 \quad (364)$$

while the lower polariton energy $E^n_a$ is real provided that

$$\tau \leq 1 \quad (365)$$

It can also be shown that $H^{\alpha, 2,n}_{\theta} = H^{\alpha, 2,a}_{\theta}$ for $\tau = 1$. Thus, as $\rho d^2$ is increased, a unique phase transition is predicted to occur at the critical point $\tau = 1$ in parameter space, beyond which the normal phase Hamiltonian, $H^{\alpha, 2,n}_{\theta}$ breaks down and the abnormal phase Hamiltonian, $H^{\alpha, 2,a}_{\theta}$, takes over. This prediction is gauge-invariant.

It now remains only to determine the nature of the unique phase transition predicted. To demonstrate equivalence between all gauges the $\alpha$-gauge transverse polarisation $P^\alpha_{\Gamma, \alpha} = \alpha_\Gamma \cdot P_T = \alpha_\Gamma (\Pi - \Pi_1)$ is calculated. In the normal phase the thermodynamic limit of this quantity, denoted $P^\alpha_{\Gamma, \alpha}$, vanishes, whereas in the abnormal phase it is found to be

$$P^\alpha_{\Gamma, \alpha} = -\alpha_\Gamma \rho d \sqrt{1 - \tau^2}. \quad (366)$$

It can be further shown that in the thermodynamic limit one obtains

$$\Pi^\alpha_{\Gamma, \alpha} = -P^\alpha_{\Gamma, \alpha}. \quad (367)$$

Therefore, choosing $\alpha = 0$ we have $-E^a_{\Gamma, \alpha} = \Pi^a_{\Gamma, \alpha} = 0$, and so we see that Eq. (367) simply expresses the fundamental kinematic relation $\Pi = -E_T - P_T$. This establishes consistency between all gauges. Independent of the gauge, the onset of the abnormal phase manifests in the form of a macroscopic value of the gauge-invariant field $P_T$:

$$P^a_{\Gamma, \alpha} = P^a_{\Gamma1, \alpha} = -\alpha_\Gamma \rho d \sqrt{1 - \tau^2}. \quad (368)$$

Previous no-go and counter no-go results can be reconciled by noting that radiation is gauge-relative. In the Coulomb gauge radiation is defined by $\Pi = -E_T$, such that the phase transition does not appear superradiant in character and only the “material” subsystem acquires a macroscopic population. This constitutes a “no-go theorem” for superradiance defined relative to the Coulomb-gauge. In the multipolar gauge radiation is defined by $\Pi = -E_T - P_T$ such that both the material and radiative subsystems acquire macroscopic population in the abnormal phase. This constitutes a “counter no-go theorem” for superradiance defined relative to the multipolar-gauge. Clearly these results are not in contradiction, because they are referring to different definitions of radiation. Indeed, the results above demonstrate that they are in fact equivalent [6]. More generally, since $\Pi = -E_T - P_T$, as expressed by Eq. (367), the degree to which the unique phase transition is classed as superradiant is directly determined by the value of $\alpha$.

We conclude by remarking that, as we have seen, $\alpha$ controls how the longitudinal electric degrees of freedom $E_i = P_T$ are shared out, thereby controlling the balance between localisation and electrostatic dressing in defining the quantum subsystem called “matter”. In Sec. V D1 we observed that the electrostatic field $P_T$ is highly localised at the position of the dipole within the approximations made and the one-dimensional model adopted. As discussed in Secs. V D1 and V D2, the answer to the question of which predictions are most relevant, i.e., to the question of whether a macroscopic average of a given property will be observed, depends on which observables are accessible via the preparation and measurement protocols available.

### 4. Extra-cavity fields

Finally, we very briefly discuss outlook for the description of external coupling to the cavity. Here we are again faced with two problems outside of traditional regimes. The first concerns the determination of which approximations might be applied and when, and the second concerns the determination of which physical states and observables are relevant in preparation and measurement.

Although the two problems are not unrelated let us consider the first problem first. For weakly coupled subsystems dissipation and decoherence can be modelled via separate loss mechanisms as though the subsystems are uncoupled. This constitutes the so-called local approach to deriving a master equation for the matter-cavity system. For example, the stationary state of a qubit in a cavity described by the local master equation

$$\dot{\rho} = -i[H, \rho] + \Gamma_1 (2\sigma^- \rho \sigma^+ - \{\sigma^+ \sigma^-, \rho\}) + \frac{\kappa}{2} (2a \rho a^\dagger - \{a^\dagger a, \rho\}) \quad (369)$$

is simply $|g, 0\rangle$. Here $\sigma^+ = |e\rangle \langle g|$ is the qubit raising operator, $\sigma^- = (\sigma^\dagger)^\imath$, and $a$ is the annihilation operator for the cavity. Dissipation is described in Eq. (369) by two separate Lindblad tails corresponding to the qubit and mode. In the so-called global approach dissipation is instead described in the dressed basis of the light-matter system.

The difference between local and global approaches has been discussed extensively and in various contexts [71, 140–160]. Cresser noted early on that the local master equation could apparently breakdown when describing a lossy Jaynes-Cummings model [161].
found by comparison with exact predictions that the local equation may perform better in the weak-coupling regime while the global master equation is generally better in the strong-coupling regime [162]. However, the relative validity of the two approaches depends on the form of secular approximation used. Cattaneo et al. have shown that the global master equation with partial secular approximation is always most accurate when Born–Markov approximations are also valid [160]. The local approach is often claimed to fail [145, 151, 154], but it has been shown to be thermodynamically consistent for fairly large ranges of coupling strengths [146, 162].

Here we note that since the gauge-parameter $\alpha$ selects the form of the interaction, one would not expect the relative applicability of local versus global master equations to be independent of $\alpha$. In general, losses of a light-matter system will depend on how it couples to the external system or environment [68, 69]. For example, Ref. [65] applies input-output theory to quantum wells within a microcavity, such that the cavity couples to external photonic modes via a number-conserving interaction while the electronic system couples to another bosonic environment similarly. With this treatment it is predicted that ground state “virtual” cavity and electronic excitations cannot leak out of the cavity. In contrast, Ref. [163] used a form of non-Markovian master equation to describe a two-level system coupled to radiation while assuming fast modulation of the vacuum Rabi frequency. It was predicted that extra-cavity quantum radiation would occur for state-of-the-art circuit cavity QED systems.

Predictions such as those in Refs. [65, 163] are in general specific to the forms of coupling adopted, i.e., they are specific to the physical subsystems considered. Indeed, as we have noted the second task that we are faced with is identifying which states and observables are relevant. If counter-rotating terms are non-negligible in the interaction of a light-matter system then the local master equation description of its losses will result in photon generation in the environmental vacuum [164]. This would typically be taken as indicating the onset of the regime in which the bare states are no longer meaningful, such that one should switch to a global description in which dissipation is described holistically using the dressed states of the full light-matter Hamiltonian [3, 68, 69, 165]. Similarly, a coarse-grained projection onto the vacuum state, as in the Born approximation, will induce apparently paradoxical spontaneous excitations in polaritonic systems. The paradox is resolved by accounting for correlations between the dressed ground state of the system and the environmental vacuum within the reservoir correlation functions of the master equation [67].

If we are interested in determining measurement signals from a source then the generic problem consists of two multi-level systems, a source and a detector, coupled to a common reservoir as was considered in Sec. V B 2. However, the multi-level source need not be elementary. In particular, it could be an ultrastrongly coupled light-matter composite. In a “global approach”, the light-matter composite is diagonalised and then weakly-coupled to whatever is external [3, 68, 69]. In this case all weak-coupling results for loss and detection are recovered with the only difference being that the eigenstates of the source are the dressed states of a composite. As previously discussed, in this context there is obviously a balance to be struck between electromagnetic dressing and localisation in spacetime. This balance is affected by the choice of gauge. The present article has focused on general aspects of light-matter interactions outside of standard regimes by examining simple setups and models. The features identified are expected to be important generally and thereby also apply to more complex systems and their reservoirs.

VI. CONCLUSIONS

In this article we have focussed on the implications of gauge-freedom for QED beyond conventional weak-coupling and Markovian regimes. We have shown that subsystems in QED are fundamentally gauge-relative meaning that in each different gauge they are defined in terms of different physical observables. The fundamental condition known as gauge-invariance states that the predictions for any physical observable must always be the same when found in different gauges. This is guaranteed by the unitarity of gauge-fixing transformations. However, if we compare predictions coming from different gauges of quantum subsystem properties such as “photon” number or “light”-“matter” entanglement, then we are comparing predictions for different physical observables which are, of course, different. This is not a violation of gauge-invariance. It is analogous to the fact that an interval in space or time between two events possesses a different value in different inertial frames, even though the same labels “space” and “time” are used in every inertial frame.

Subsystem gauge-relativity can be ignored within the idealised setting of scattering theory, beyond which it can only be eliminated using various weak-coupling and Markovian approximations. It is therefore an important fundamental feature whenever such approximations cannot be employed, i.e., outside of gauge non-relativistic regimes. We have provided descriptions of a number of simple systems, showing that subsystem gauge-relativity is significant in the description of so-called “virtual” processes. It thereby affects the balance between localisation and electromagnetic dressing. This has non-trivial implications for modelling controllable interactions, for photodetection theory, and for cavity QED. In all instances, the quantum subsystems, including reservoirs and measurement devices, can only be defined relative to a choice of gauge. Beyond conventional weak-coupling and Markovian regimes the physical predictions for subsystems defined relative to different gauges can be markedly different.
Appendix: Gauge-freedom in material polarisation and gauge-fixing

When writing the physical electromagnetic fields in terms of a scalar potential $A_0$ and vector potential $\mathbf{A}$ a gauge-freedom occurs. A similar freedom also occurs when writing the physical material charge and current densities $\rho$ and $\mathbf{J}$ in terms of the auxiliary polarisation $\mathbf{P}$ and magnetisation $\mathbf{M}$. These fields can be defined by the inhomogeneous Maxwell equations;

$$\rho = -\nabla \cdot \mathbf{P}, \quad \mathbf{J} = \dot{\mathbf{P}} + \nabla \times \mathbf{M}. \quad (370)$$

In the absence of any accompanying homogenous Maxwell equations the fields $\mathbf{P}$ and $\mathbf{M}$ are not unique. Specifically, the physical charge and current densities are invariant under a transformation by pseudo-magnetic and pseudo-electric fields as

$$\mathbf{P} \rightarrow \mathbf{P} + \nabla \times \mathbf{U}, \quad \mathbf{M} \rightarrow \mathbf{M} - \nabla U_0 - \dot{U} \quad (371)$$

where $U$ is an arbitrary pseudo-four-potential. The fields are in turn invariant under a gauge-transformation $U_\mu \rightarrow U_\mu - \partial_\mu \chi$ where $\chi$ is arbitrary.

The polarisation field is obtained by inverting the divergence operator $[4, 6]$

$$\mathbf{P}(\mathbf{x}) := -\int d^3x' \mathbf{g}(\mathbf{x}, \mathbf{x}')\rho(\mathbf{x}'), \quad (372)$$

$$\nabla \cdot \mathbf{g}(\mathbf{x}, \mathbf{x}') = \delta(\mathbf{x} - \mathbf{x}'). \quad (373)$$

It therefore has completely arbitrary transverse component as already expressed by Eq. (371). In conventional approaches to non-relativistic QED all gauge redundancies are eliminated simultaneously as described below.

In Sec. II B the gauge-fixing constraint imposed is [cf. Eqs. (44) and (45)]

$$\int d^3x' \mathbf{g}(\mathbf{x}', \mathbf{x}) \cdot \mathbf{A}(\mathbf{x}') = 0. \quad (374)$$

where $\mathbf{g} = \mathbf{g}_r + \mathbf{g}_l$ with

$$\mathbf{g}_l(\mathbf{x}, \mathbf{x}') := -\nabla \frac{1}{4\pi|\mathbf{x} - \mathbf{x}'|}. \quad (375)$$

and with $\mathbf{g}_r$ arbitrary, such that the choice of $\mathbf{g}_r$ determines the gauge. In Sec. II A this choice is restricted by imposing that $\mathbf{g}_r = \mathbf{g}_{r\alpha}$ where

$$g_{r\alpha}(\mathbf{x}, \mathbf{x}') := -\alpha \int_0^1 d\lambda \mathbf{x}_\lambda^\prime \delta_{\nu}^\lambda(\mathbf{x} - \lambda \mathbf{x}'). \quad (377)$$

The $\alpha$-gauge polarisation field is then $[4, 6]$

$$\mathbf{P}_{r\alpha}(\mathbf{x}) := -\int d^3x' \mathbf{g}_{r\alpha}(\mathbf{x}, \mathbf{x}')\rho(\mathbf{x}'). \quad (378)$$

A choice of $\alpha$ completely determines $\mathbf{g}_r$ which then uniquely determines the vector and scalar potentials as well as the material polarisation.

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