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Reply to: Gauge non-invariance due to material truncation in ultrastrong-coupling quantum electrodynamics

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REPLYING TO Stokes, A. & Nazir, A. *Nature Physics* https://doi.org/10.1038/s41567-023-02155-8 (2023)

In their Matters Arising[1], Stokes and Nazir point out that the main text of ref. 2 did not explicitly define the unitary operator $\hat{\mathcal{U}}$ as: $\hat{\mathcal{U}} = \hat{U}(\hat{P}x\hat{P})$, where x is the coordinate of the effective particle and

$$\hat{P} = \hat{I}_2 = |0\rangle\langle 0| + |1\rangle\langle 1|\,, \tag{1}$$

is the identity for the truncated Hilbert space (see the text below equation (5) in ref. 2). As can be inferred from both equation (9) and Section I of the Supplementary Information of ref. 2, all our results in the correct Coulomb gauge have been obviously obtained using the unitary operator $\hat{\mathcal{U}} = \hat{U}(\hat{P}x\hat{P})$.

The equivalence $\hat{P}\hat{U}\hat{P} = \hat{U}(\hat{P}x\hat{P})$ was a direct consequence of the adopted truncation procedure described in ref. 2. Specifically, (1) in ref. 2 the Hilbert space truncation occurs once and definitely, and the light–matter interaction is introduced only after the Hilbert space truncation. When the matter system is described by a two-level atom, any meaningful operator has to be an endomorphism in the truncated Hilbert space, and the standard properties of identity operators can be legitimately used for $\hat{P}$ in equation (1); (2) the equivalence $\hat{P}\hat{U}\hat{P} = \hat{U}(\hat{P}x\hat{P})$ can be obtained by expanding $\hat{U}(x)$ in a Taylor series and then using for each term the relation $\hat{P}x^n\hat{P} = (\hat{P}x\hat{P})^n$, which can be easily obtained using the properties of identity operators (Section 1 of the Supplementary Information in ref. 2); and (3) the definition of $\hat{P}$ (equation (1)) after the truncation, used throughout the paper[2], is very clearly stated already below equation (5) in ref. 2. Stokes and Nazir incorrectly attribute to us their definition of $\hat{P}$[1] as an operator living in an infinite-dimensional Hilbert space, instead of our two-dimensional Hilbert space.

Gauge invariance or gauge principle?

In ref. 1 the authors define x_P-phase invariance as the invariance based on the truncated finite-dimensional position operator. However, their definition expresses a rather different concept with respect to the gauge principle in the truncated spaces introduced in ref. 2 and to the implementation of this principle in lattice gauge theories (LGT)[3–5].

After the authors of ref. 1 introduce their own definition of x_P-phase invariance, then they claim that every truncated model possesses this property (their definition), including all those given in refs. 6,7. Hence, according to the authors of ref. 1, x_P-phase invariance cannot determine the correct light–matter interaction. If their definition were to agree with the general concept of the gauge principle (as in LGT), their demonstration would put into question not only the results in ref. 2, but also LGT, one of the most advanced and broadly employed tools in quantum field theory. However, this is not the case as we show below.

Specifically, we find that their conclusion, that every truncated model possesses x_P-phase invariance (including all those given in refs. 6,7, wherein gauge non-invariance due to truncation was identified), is just a consequence of their own specific definition. We show here that, in contrast to the Hamiltonian in equation (11) of ref. 2, the models given in refs. 6,7 (except the dipole gauge Hamiltonian) do not satisfy the physically meaningful gauge principle for truncated models.

In quantum mechanics and specifically in quantum field theory, the coupling of particles with fields is constructed in such a way that the theory is invariant under local transformations (gauge principle) (for example, ref. 8). For example, considering $U(1)$ invariance, the Dirac action is not invariant under local phase transformations of the wave function: $\psi(x) \to \exp[iq\theta(x)]\psi(x)$, where i is the imaginary unit, q is charge, and $\theta(x)$ is a position-dependent phase. It is well-known that invariance can be restored by replacing all derivatives ∂_μ in the Lagrangian with covariant derivatives $D_\mu \equiv \partial_\mu + iqA_\mu$, where A_μ are components of the field coordinate, which transform as $A_\mu \to A_\mu - \partial_\mu\theta$.

In approximated models where the space is no longer continuous, as in truncated Hilbert spaces, transformations involving phases depending on continuous coordinates are no longer meaningful, and can give rise to ambiguities in the choice of the light–matter model[6]. However, in these cases, it is possible to define a position operator with

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discrete eigenvalues, as in LGT. Hence, continuous phase transformations become unitary transformations of phases which are defined at discrete points. The general procedure to build gauge-invariant theories for truncated Hilbert spaces is unambiguous and rather clear: one starts from the Lagrangian (or even from the Hamiltonian in some cases) of the matter system in the truncated space, then introduces the coupling with a field able to restore the phase invariance in the truncated space. This is just the philosophy of LGT. On the contrary, the x_P-phase invariance introduced in ref. 1 starts from a gauge dependent (α) Hamiltonian, and then applies an (α') transformation. These mathematical transformations are not physically related to the gauge principle, because these are applied to Hamiltonians that already include the concept of light–matter interaction. The gauge principle applies to matter systems only to introduce the field–matter interaction as a mechanism to restore local invariance, starting from a Lagrangian for the matter system which does not include the gauge field[8].

It can be shown that the Coulomb gauge Hamiltonian in ref. 2 corresponds to a two-site version of an abelian (non-relativistic) LGT. According to these gauge theories, if a state is defined on a discrete set of points, a meaningful and consistent local phase transformation cannot be a continuous function $\theta(x)$. It will be a discrete set θ_i, where i labels the lattice points. Considering, for example, a particle in an even potential with two separated minima, it is possible to define two localized states ($|R\rangle$ and $|L\rangle$) as

$$|R(L)\rangle = \frac{1}{\sqrt{2}}(|0\rangle \pm |1\rangle), \tag{2}$$

where $\{|0|\rangle, |1\rangle\}$ are the two lowest-energy eigenstates. The two-level system Hamiltonian can be written as

$$\hat{\mathcal{H}}_0 = -t\, |R\rangle\langle L| + \text{h.c.} \tag{3}$$

h.c. indicates hermitian conjugate. Considering a generic state $|\psi\rangle = c_L\,|L\rangle + c_R\,|R\rangle$, the expectation values of $\hat{\mathcal{H}}_0$ are not invariant under the local phase transformations: $c_{L(R)} \to c_{L(R)} \exp\{i\theta_{L(R)}\}$. Gauge invariance is restored introducing Wilson's parallel transporter $U_{L-R} = \exp\{iqaA\}$, where q is the charge, $a = 2\langle 1|\,x\,|0\rangle$, and A is the vector potential calculated at the atom position (dipole approximation):

$$\hat{\mathcal{H}}_0 \to \hat{\mathcal{H}}_0^{\text{gi}} = -t\, |R\rangle\langle L|\, e^{iqaA} + \text{h.c.} \tag{4}$$

After some algebra, it results that just adding the free-field term to this Hamiltonian gives equation (10) in ref. 2.

Further details can be found elsewhere[9]. On the contrary, other quantum Rabi models[1] not connected by unitary transformations to equation (4) violate the gauge principle and gauge invariance for two-level systems.

In addition, we highlight some relevant, general and well-known features of gauge theories: (1) the operators determining the transformations of particle states are elements of a representation of a Lie group, and the group properties are essential to make these transformations meaningful; (2) the transformed states have to belong to the same Hilbert space of the initial states; and (3) Lie algebra implies that in the neighbourhood of the identity element, the generic element of the representation can be expanded as $\hat{D}(\theta) \simeq \hat{I} + i\theta_a \hat{T}_a$, where θ_a are continuous parameters and $\hat{T}_a$ the generators of the group. The generic group elements can then always be represented by $\hat{D}(\theta) = \exp(i\theta_a \hat{T}_a)$. In our case $\hat{T}_a \propto \hat{x}_p$ (Section 1 of Supplementary Information in ref. 2).

According to ref. 6, the procedure performed in ref. 2 amounts to truncating the multipolar gauge followed by rotation within the truncated space. Instead, we have just shown that the Hamiltonian equation (10) in ref. 2 corresponds to what is obtained from the only physically meaningful implementation of the gauge principle in truncated Hilbert spaces in agreement with LGT. Hence, the opposite view is more suited: the multipolar quantum Rabi model works fine because it can be directly obtained by a proper gauge (unitary) transformation from the two-level model satisfying the gauge principle in truncated models, in agreement with LGT. Note that LGTs[3,5], as well as the related Peierls substitution[10] were developed to implement the minimal coupling replacement in a lattice without any reference to the multipolar gauge.

Conclusion

In summary, we have shown that the first argument of ref. 1, claiming that the results of ref. 2 are not valid, is not correct. The second criticism is that the gauge principle in the truncated Hilbert space (x_P-phase invariance) is not able to provide the correct model of the light–matter interaction Hamiltonian, since several models can satisfy this principle. If this claim were correct, it would put into question not only the results in ref. 2, but also LGT, one of the most advanced and broadly employed tools in quantum field theory. However, the conclusion of the second argument of ref. 1 is just the direct consequence of their own specific definition, unrelated to the approach of ref. 2 and to the general gauge principle in LGTs, which is the natural and consistent extension of the gauge principle in the presence of discrete coordinates. We have shown that the main argument of the comment[1] has no physical meaning and it is inconsistent with the gauge principle.

Online content

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Please detail the contributions of all authors here.

Competing interests

The authors declare no competing interests.

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